On the physical part of the factorized correlation functions of the XXZ chain

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Abstract

It was recently shown by Jimbo, Miwa and Smirnov that the correlation functions of a generalized XXZ chain associated with an inhomogeneous six-vertex model with disorder parameter α and with arbitrary inhomogeneities on the horizontal lines factorize and can all be expressed in terms of only two functions ρ and ω. Here we approach the description of the same correlation functions and, in particular, of the function ω from a different direction. We start from a novel multiple integral representation for the density matrix of a finite chain segment of length m in the presence of a disorder field α. We explicitly factorize the integrals for $m = 2$. Based on this we present an alternative description of the function ω in terms of the solutions of certain linear and nonlinear integral equations. We then prove directly that the two definitions of ω describe the same function. The definition in the work of Jimbo, Miwa and Smirnov was crucial for the proof of the factorization. The definition given here together with the known description of ρ in terms of the solutions of nonlinear integral equations is useful for performing e.g. the Trotter limit in the finite temperature case, or for obtaining numerical results for the correlation functions at short distances. We also address the issue of the construction of an exponential form of the density matrix for finite α.

PACS: 05.30.-d, 75.10.Pq

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1 Introduction

In recent years significant progress has been achieved in the understanding of the mathematical structure of the correlation functions of the XXZ model and related integrable models. First of all the ground state correlation functions were studied. They are completely defined through the quantum-mechanical density matrix. An explicit expression for the density matrix of a finite subchain of the infinite XXZ chain in the massive regime was first obtained by Jimbo, Miki, Miwa and Nakayashiki [17]. They expressed the elements of the density matrix in terms of multiple integrals. Subsequently, extensions of their formulae to the massless regime and to a non-vanishing longitudinal magnetic field were obtained in [18, 22].

Then it was realized that the multiple integrals can be factorized [10] and that, utilizing the so-called reduced Knizhnik-Zamolodchikov equation, the factorized integrals can be written in a compact exponential form [6, 7]. The latter allows one to distinguish between an algebraic part and a physical part. The physical part is defined by a small number of transcendental functions, fixed by the one-point-correlators and by the two-point neighbour correlators which depend on the physical parameters like anisotropy, temperature, length of the chain, magnetic field, boundary conditions etc. The algebraic part is related to the representation theory of the symmetry algebra behind the model, namely the quantum group $U_q(\widehat{\mathfrak{sl}_2})$ in case of the XXZ chain.

In [8] it was observed that the formula for the correlation functions looks nicer if the XXZ chain is regularized by introducing an additional parameter, the disorder field α. With this new parameter it was possible to express the density matrix in terms of special fermionic annihilation operators $\mathbf{b}$ and $\mathbf{c}$ acting not on states of the spin chain, but on the space of (quasi-) local operators on these states. The annihilation operators appeared to be responsible for the algebraic part. The physical part was represented by a transcendental function ω determined by a single integral. In [9] the dual fermionic creation operators $\mathbf{b}^*$, $\mathbf{c}^*$ and a bosonic creation operator $\mathbf{t}^*$ were constructed. These operators together generate a special basis of the space of quasi-local operators. Since $\mathbf{b}^*$, $\mathbf{c}^*$ are Fermi operators, Wick's theorem applies and expectation values of products of $\mathbf{b}^*$, $\mathbf{c}^*$ and $\mathbf{t}^*$ in an appropriately defined vacuum state can be written as determinants, very much as in the case of free fermions.

Thermodynamic properties of integrable lattice models can be studied within the Suzuki-Trotter formalism by considering an auxiliary lattice with staggering in the so-called Trotter direction [24]. The temperature appears as a result of a special limit when the extension of the lattice in Trotter direction becomes infinite. Physical quantities are expressed in an efficient way through the solution to certain non-linear integral equations [23]. A detailed discussion of this issue and further references can, for instance, be found in the book [12].

In papers [14, 15] the Suzuki-Trotter formalism was used in order to generalize the multiple integrals to finite temperature. Then their factorization was probed for several examples of correlation functions, first for the XXX chain [3] and later for the XXZ chain [2, 4]. Also a conjecture was formulated stating that the above mentioned exponential form is valid with the same fermionic operators (at least as long as they act on spin reversal invariant products of local operators) as for the ground state and

two functions ω, ω' obtained from an α-dependent function in the limit $\alpha \to 0$.

Unfortunately, the formulae of [2, 4] worked only in this limit. The generalization to generic α stayed obscure. One of the purposes of the present work is to add to the clarification of this point, starting from a proper multiple integral representation with disorder parameter α. Here, as we had to learn [20], the crucial point is that the 'Cauchy extraction trick', invented in [16] and described in more detail in [21], can be applied in the finite temperature case and also in the more general situation of a finite lattice with inhomogeneities in Trotter direction.

Important new insight came from a recent paper [19] by Jimbo, Miwa and Smirnov, where they suggested a purely algebraic approach to the problem of calculating the static correlation functions of the XXZ model. The key idea of [19] is to evaluate a linear functional related to the partition function within the fermionic basis constructed in [9]. The authors of [19] work with a finite lattice, inhomogeneous in Trotter direction. In this situation they suggest a new and surprising construction of the function ω depending on a magnetic field and on the disorder parameter α.

In the present paper we discuss the relation of the work by Jimbo, Miwa and Smirnov to the approach using non-linear integral equations which at the moment seems more appropriate e.g. for taking the Trotter limit (which was omitted in [19]). In particular, we present an alternative description of the function ω starting from the multiple integral and using the explicit factorization of the density matrix for two neighbouring lattice sites. We then give a direct proof that our expression, though looking rather different than that in [19], in fact describes the same function.

An inhomogeneous lattice in Trotter direction is very general and leaves many different options for the realization of physical correlation functions. Here we shall concentrate on two of them, the correlation functions of the infinite XXZ chain at finite temperature and magnetic field (temperature case) and the ground state correlation functions of a finite chain with twisted periodic boundary conditions (finite length case). Both cases can be treated to a very large extend simultaneously. They are only distinct in that a different distribution of inhomogeneity parameters is required and in that for the finite temperature case the Trotter limit has to be performed. Note that instead of the XXZ Hamiltonian we could consider combinations of conserved quantities obtained from the transfer matrix of the six-vertex model within the formalism of non-linear integral equations. For the bulk thermodynamic properties this issue was recently studied in [25].

The paper is organized as follows. In the next section we define our basic objects and recall some of their properties. In the third section we show the multiple integral formula for the elements of the (α-twisted) density matrix for a sub-chain of length m. In section four we consider the simplest case $m = 1$. The fifth section is devoted to applying the factorization technique to the double integrals for $m = 2$. In section 6 we introduce the function ω. We discuss its properties and the relation to its realization by Jimbo, Miwa and Smirnov. The content of section 7 is some preliminary work on the construction of an operator $\mathbf{t}$, dual to the creation operator $\mathbf{t}^*$, which should appear in the construction of an exponential form for finite temperature and finite disorder parameter. In the appendices we provide a derivation of the multiple integral formulae, we discuss the limit $\alpha \to 0$, and we compare with the results of the papers [2, 4].

2 Density matrix and correlation functions

The XXZ quantum spin chain is defined by the Hamiltonian

$$H_N(\kappa) = J \sum_{j=1}^{N} \big(\sigma_{j-1}^x \sigma_j^x + \sigma_{j-1}^y \sigma_j^y + \Delta(\sigma_{j-1}^z \sigma_j^z - 1)\big)\,, \tag{1}$$

written here in terms of the Pauli matrices $\sigma^x = e_-^+ + e_+^-$, $\sigma^y = \mathrm{i}(e_-^+ - e_+^-)$, $\sigma^z = e_+^+ - e_-^-$ (where the e_β^α are the elements of the gl(2) standard basis). The two real parameters J and Δ control the ground state phase diagram of the model. For simplicity of notation we shall restrict ourselves in the following to the critical phase $J > 0$, $|\Delta| < 1$. Note, however, that the results of this work can be easily extended to the off-critical antiferromagnetic phase $\Delta > 1$. We shall also assume without further mentioning that the number of lattice sites N is even.

To fully specify $H_N(\kappa)$ we have to define the boundary conditions. We shall consider twisted periodic boundary conditions, when we are dealing with the ground state of the finite chain. Then $H_N(\kappa)$ depends on an additional parameter κ through

$$\begin{pmatrix} e_0{}_+^+ & e_0{}_-^+ \\ e_0{}_+^- & e_0{}_-^- \end{pmatrix} = q^{-\kappa\sigma^z} \begin{pmatrix} e_N{}_+^+ & e_N{}_-^+ \\ e_N{}_+^- & e_N{}_-^- \end{pmatrix} q^{\kappa\sigma^z}\,. \tag{2}$$

Here q is related to Δ as $\Delta = (q + q^{-1})/2$. For the finite temperature case we shall assume periodic boundary conditions for the Hamiltonian. Nevertheless the same parameter κ will appear in that case as a twist parameter of the quantum transfer matrix, having then a rather different physical meaning as an external magnetic field coupling to the spins by a Zeeman term. We shall elaborate on this below.

The integrable structure behind the Hamiltonian (1) is generated by the trigonometric R-matrix of the six-vertex model [1],

$$R(\lambda) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & b(\lambda) & c(\lambda) & 0 \\ 0 & c(\lambda) & b(\lambda) & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}\,, \tag{3}$$

$$b(\lambda) = \frac{\mathrm{sh}(\lambda)}{\mathrm{sh}(\lambda+\eta)}\,, \quad c(\lambda) = \frac{\mathrm{sh}(\eta)}{\mathrm{sh}(\lambda+\eta)}\,, \tag{4}$$

acting on $\mathbb{C}^2 \otimes \mathbb{C}^2$. As presented here it satisfies the Yang-Baxter equation in additive form. To facilitate the comparison with [9, 19], where the multiplicative form was preferred, we set $q = \mathrm{e}^\eta$ and $\zeta = \mathrm{e}^\lambda$. Then for arbitrary complex inhomogeneity parameters β_j, $j = 1, \dots, N$, the definition

$$T_a(\zeta) = R_{a,N}(\lambda - \beta_N) \dots R_{a,1}(\lambda - \beta_1) \tag{5}$$

of the monodromy matrix makes sense, where, as usual, the indices $1, \dots, N$ refer to the spin chain while a refers to an additional site defining the so-called auxiliary space. We also set $T_a(\zeta,\kappa) = T_a(\zeta) q^{\kappa\sigma_a^z}$ and introduce the twisted transfer matrix

$$t(\zeta,\kappa) = \mathrm{tr}_a\big(T_a(\zeta,\kappa)\big)\,. \tag{6}$$

In [19] a six vertex-model with N horizontal rows and an arbitrary distribution of the inhomogeneities $\tau_j = \mathrm{e}^{\beta_j}$ on these rows was considered. Here we would like to point out that two specific distributions are of particular interest in physical applications. Moreover, in both cases the special functions that enter the representations of the transfer matrix eigenvalues and correlation functions have nice descriptions in terms of solutions of linear and non-linear integral equations.

The first case relates to the ground state of the Hamiltonian (1). We call it the finite length case. In this case we choose

$$\beta_j = \eta/2\,, \quad j = 1,\dots,N\,. \tag{7}$$

Then

$$H_N(\kappa) = 2J\,\mathrm{sh}(\eta)\,\partial_\lambda \ln\bigl(t^{-1}(q^{\frac{1}{2}},\kappa)\,t(\zeta,\kappa)\bigr)\big|_{\lambda=\eta/2}\,, \tag{8}$$

with twisted boundary conditions (2) if we identify $\Delta = \mathrm{ch}(\eta)$. The critical regime $|\Delta| < 1$ corresponds to purely imaginary $\eta = \mathrm{i}\gamma$, $\gamma \in [0,\pi)$. In this case the physical twist angle or flux $\Phi \in [0,2\pi)$ is $\Phi = -\kappa\gamma$, whence κ should be real. If we stick to the vertex model picture of [19], then $t(\zeta,\kappa)$ is the vertical or column-to-column transfer matrix in this case.

The second case is determined by an alternating choice

$$\beta_j = \begin{cases} \beta_{2j-1} = \eta - \frac{\beta}{N} \\ \beta_{2j} = \frac{\beta}{N} \end{cases}, \quad j = 1,\dots,N/2\,, \tag{9}$$

of inhomogeneity parameters. This case will be called the finite temperature case as it relates to the quantum transfer matrix, whose monodromy matrix is

$$T_a^{QTM}(\zeta) = \\ R_{a,N}(\lambda-\beta/N)R^{t_1}_{N-1,a}(-\beta/N-\lambda)\dots R_{a,2}(\lambda-\beta/N)R^{t_1}_{1,a}(-\beta/N-\lambda)\,. \tag{10}$$

Here the superscript 't_1' indicates transposition with respect to the first space. In fact, setting $Y = \prod_{j=1}^{N/2}\sigma^y_{2j-1}$ and using the crossing symmetry

$$\sigma^y_j R_{a,j}(\lambda-\eta)\sigma^y_j = b(\lambda-\eta)R^{t_1}_{j,a}(-\lambda) \tag{11}$$

of the R-matrix we find that

$$T_a^{QTM}(\zeta) = Y\,T_a(\zeta)\,Y\prod_{j=1}^{N/2}\frac{1}{b(\lambda-\beta_{2j-1})}\,. \tag{12}$$

The quantum transfer matrix is by definition

$$t^{QTM}(\zeta,\kappa) = \mathrm{tr}_a\bigl(T_a^{QTM}(\zeta,\kappa)\bigr)\,, \tag{13}$$

where $T_a^{QTM}(\zeta,\kappa) = T_a^{QTM}(\zeta)q^{\kappa\sigma^z_a}$.

Again, within the vertex model picture, $t^{QTM}(\zeta,\kappa)$, or $t(\zeta,\kappa)$ with the choice (9) of inhomogeneity parameter, corresponds to the vertical transfer matrix. There is an

important difference, though, that has been explained at several occasions [14, 23]. In the finite length case the Hamiltonian can be derived from the vertical transfer matrix. In particular, the vertical transfer matrix and the Hamiltonian (1) have the same eigenstates. In the finite temperature case, on the other hand, with a lattice which is homogeneous in horizontal direction, say, the Hamiltonian is related to the horizontal transfer matrix with purely periodic boundary conditions. It is then also periodic and will be denoted $H_L(0)$, where L is the horizontal extension of the lattice. In this case the vertical transfer matrix eigenstates are different from those of the Hamiltonian. In particular, the eigenstate with the largest modulus determines the state of thermodynamic equilibrium in the thermodynamic limit, i.e. the free energy of the XXZ chain and all its static correlation functions [14]. Also the physical interpretation of the parameter κ is rather different in this case. It corresponds to a magnetic field coupling to the spin chain through a Zeeman term (see e.g. [14]).

Using a lattice of finite extension L in horizontal direction we can express the partition function of the homogeneous XXZ chain of length L as

$$Z_L = \mathrm{tr}_{1,\dots,L}\, \mathrm{e}^{-\beta H_L(0) + hS_{[1,L]}/T} = \lim_{N\to\infty} \mathrm{tr}_{1,\dots,N} \left(t^{QTM}(1, h/(2\eta T))\right)^L . \tag{14}$$

Here T is the temperature and h is a longitudinal magnetic field. β must be chosen as $\beta = 2J\,\mathrm{sh}(\eta)/T$. Furthermore

$$S_{[1,L]} = \tfrac{1}{2}\sum_{j=1}^{L} \sigma_j^z \tag{15}$$

is the conserved z-component of the total spin. Equation (14) becomes efficient in the thermodynamic limit $L \to \infty$, since then a single eigenvalue $\Lambda^{QTM}(1,\kappa)$ of $t^{QTM}(1,\kappa)$ of largest modulus dominates the large-L asymptotics of Z_L in the Trotter limit $N \to \infty$. We shall refer to this eigenvalue as the dominant one.

We would like to remark that in our understanding the quantum transfer matrix is, in general, more appropriate for studying integrable spin models on the infinite lattice than the usual transfer matrix. In general there is no crossing symmetry, and the quantum transfer matrix and the usual transfer matrix are not related by a similarity transformation like in (12). Also within the quantum transfer matrix formulation the density matrix directly takes its 'natural form' in terms of monodromy matrix elements (see below). No solution of a quantum inverse problem as in [22] is required. In our particular case we do have the crossing symmetry, and the quantum transfer matrix and the usual transfer matrix with staggered inhomogeneities (9) give an equivalent description of the density matrix (see below). Still, the largest eigenvalue of $t(\zeta,\kappa)$ with the distribution (9) of inhomogeneities diverges in the Trotter limit as can be seen from (12).

Let us come back to the situation of arbitrarily distributed inhomogeneity parameters β_j. Following [19] we shall assume that for a certain spectral parameter ζ_0 and any $\kappa \in \mathbb{C}$ the transfer matrix $t(\zeta_0,\kappa)$ has a unique eigenvector $|\kappa\rangle$ with eigenvalue $\Lambda(\zeta_0,\kappa)$ of largest modulus. This is certainly true for the two special cases considered above. In the finite length case $\zeta_0 = q^{1/2}$, while $\zeta_0 = 1$ in the finite temperature case. We fix a set of 'vertical inhomogeneity parameters' $\nu_1,\dots,\nu_m$ and set $\xi_j = \mathrm{e}^{\nu_j}$. Then

we can define the object of our main interest, the density matrix with matrix elements

$$D_N{}^{\varepsilon_1'\dots\varepsilon_m'}_{\varepsilon_1\dots\varepsilon_m}(\xi_1,\dots,\xi_m|\kappa,\alpha) = \frac{\langle\kappa+\alpha|T^{\varepsilon_1'}_{\varepsilon_1}(\xi_1,\kappa)\dots T^{\varepsilon_m'}_{\varepsilon_m}(\xi_m,\kappa)|\kappa\rangle}{\langle\kappa+\alpha|\prod_{j=1}^m t(\xi_j,\kappa)|\kappa\rangle}\,, \tag{16}$$

which is in fact an inhomogeneous and 'α-twisted' version of the usual density matrix.

In the finite length case (7) with twist angle Φ the expectation value in the ground state $|\Phi\rangle$ of any operator $X_{[1,m]}$ acting non-trivially only on the first m lattice sites is [11]

$$\frac{\langle\Phi|X_{[1,m]}|\Phi\rangle}{\langle\Phi|\Phi\rangle} = \lim_{\alpha\to 0}\lim_{\nu_j\to\eta/2}\mathrm{tr}_{1,\dots,m}\big\{D_N(\xi_1,\dots,\xi_m|-\Phi/\gamma,\alpha)\,X_{[1,m]}\big\}\,. \tag{17}$$

In the finite temperature case (9) we use that the right hand side of (16) stays form invariant under the transformation (12) which replaces all objects relating to the ordinary transfer matrix with the corresponding objects relating to the quantum transfer matrix. Hence, from [15],

$$\begin{aligned}\langle X_{[1,m]}\rangle_{T,h} &= \lim_{L\to\infty}\frac{\mathrm{tr}_{1,\dots,L}\big\{\mathrm{e}^{-\beta H_L(0)+hS_{[1,L]}/T}X_{[1,m]}\big\}}{Z_L}\\ &= \lim_{\alpha\to 0}\lim_{\nu_j\to 0}\lim_{N\to\infty}\mathrm{tr}_{1,\dots,m}\big\{D_N(\xi_1,\dots,\xi_m|h/(2\eta T),\alpha)\,X_{[1,m]}\big\}\,.\end{aligned} \tag{18}$$

The density matrix (16) allows for reduction from the left and from the right expressed by

$$\mathrm{tr}_1\big\{D_N(\xi_1,\dots,\xi_m|\kappa,\alpha)q^{\alpha\sigma_1^z}\big\} = \rho(\xi_1)D_N(\xi_2,\dots,\xi_m|\kappa,\alpha)\,, \tag{19a}$$

$$\mathrm{tr}_m\big\{D_N(\xi_1,\dots,\xi_m|\kappa,\alpha)\big\} = D_N(\xi_1,\dots,\xi_{m-1}|\kappa,\alpha)\,, \tag{19b}$$

where

$$\rho(\zeta) = \frac{\Lambda(\zeta,\kappa+\alpha)}{\Lambda(\zeta,\kappa)}\,. \tag{20}$$

The function ρ plays an important role in [19]. As we shall see below it is also important for the formulation of a multiple integral formula for the density matrix and is the only non-trivial one-point function for finite α. In the temperature case with $\kappa = h/(2\eta T)$ we have

$$\rho(1) = 1 + m(T,h)2\eta\alpha + \mathcal{O}(\alpha^2)\,, \tag{21}$$

where $m(T,h)$ is the magnetization.

In the temperature case as well as in the finite length case and in certain inhomogeneous generalizations of both cases the function ρ can be expressed in terms of an integral over certain auxiliary functions (see e.g. [11, 14]),

$$\rho(\zeta) = q^\alpha\exp\bigg\{\int_{\mathcal{C}}\frac{\mathrm{d}\mu}{2\pi\mathrm{i}}\,\mathrm{e}(\mu-\lambda)\ln\bigg[\frac{1+\mathfrak{a}(\mu,\kappa+\alpha)}{1+\mathfrak{a}(\mu,\kappa)}\bigg]\bigg\}\,. \tag{22}$$

Here $\mathrm{e}(\lambda)$ is the 'bare energy'

$$\mathrm{e}(\lambda) = \mathrm{cth}(\lambda) - \mathrm{cth}(\lambda+\eta) \tag{23}$$

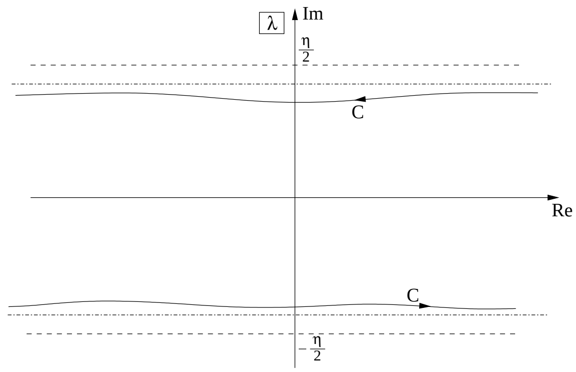

Figure 1: The canonical contour $\mathcal{C}$ surrounds the real axis in counterclockwise manner inside the strip $-\frac{\gamma}{2} < \operatorname{Im}\lambda < \frac{\gamma}{2}$.

and $\mathfrak{a}(\lambda,\kappa)$ is the solution of a non-linear integral equation with integration kernel

$$K(\lambda) = \operatorname{cth}(\lambda-\eta) - \operatorname{cth}(\lambda+\eta)\,. \tag{24}$$

In the finite length case this equation reads

$$\ln(\mathfrak{a}(\lambda,\kappa)) = \\ (N-2\kappa)\eta + \sum_{j=1}^{N} \ln\left[\frac{\operatorname{sh}(\lambda-\beta_j)}{\operatorname{sh}(\lambda-\beta_j+\eta)}\right] - \int_{\mathcal{C}} \frac{d\mu}{2\pi i} K(\lambda-\mu)\ln(1+\mathfrak{a}(\mu,\kappa))\,. \tag{25}$$

Equations (22) and (25) are still valid if the β_j are not precisely those of equation (7), but are close to $\eta/2$ with $\operatorname{Im}\beta_j = \gamma/2$. The contour of integration to be used in (22) and (25) is shown in figure 1. In the temperature case the non-linear integral equation has a similar structure, but the driving term is different. Suppose that for $j = 1,\dots,N/2$ the β_{2j-1} are close to η, whereas the β_{2j} are close to 0. Then

$$\ln(\mathfrak{a}(\lambda,\kappa)) = -2\kappa\eta \\ + \sum_{j=1}^{N/2} \ln\left[\frac{\operatorname{sh}(\lambda-\beta_{2j})\operatorname{sh}(\lambda-\beta_{2j-1}+2\eta)}{\operatorname{sh}(\lambda-\beta_{2j}+\eta)\operatorname{sh}(\lambda-\beta_{2j-1}+\eta)}\right] - \int_{\mathcal{C}} \frac{d\mu}{2\pi i} K(\lambda-\mu)\ln(1+\mathfrak{a}(\mu,\kappa))\,. \tag{26}$$

We presented both equations (25) and (26) in inhomogeneous form, since we shall need this later, when comparing with [19]. Note, however, that the homogeneous limit is trivial in both cases and that, moreover, the Trotter limit can be performed in (26). Then

$$\ln(\mathfrak{a}(\lambda,\kappa)) = (N-2\kappa)\eta + N\ln\left[\frac{\operatorname{sh}(\lambda-\eta/2)}{\operatorname{sh}(\lambda+\eta/2)}\right] - \int_{\mathcal{C}} \frac{d\mu}{2\pi i} K(\lambda-\mu)\ln(1+\mathfrak{a}(\mu,\kappa))\,. \tag{27}$$

in the finite length case and

$$\ln(\mathfrak{a}(\lambda,\kappa)) = -2\kappa\eta - \frac{2J\operatorname{sh}(\eta)e(\lambda)}{T} - \int_{\mathcal{C}} \frac{d\mu}{2\pi i} K(\lambda-\mu)\ln(1+\mathfrak{a}(\mu,\kappa)) \tag{28}$$

in the temperature case and in the Trotter limit. Equations (27) and (28) are what we call the $\mathfrak{a}$-form of the non-linear integral equation. There is another so-called $\mathfrak{b}\overline{\mathfrak{b}}$-form [11, 23] which is more convenient for an accurate calculation of the numerical values of the functions.

3 The multiple integral representation of the density matrix

In appendix A we derive the following multiple integral representation for the elements of the density matrix.

$$D_{N\,\varepsilon_1\dots\varepsilon_m}^{\varepsilon'_1\dots\varepsilon'_m}(\xi_1,\dots,\xi_m|\kappa,\alpha) = \left[\prod_{j=1}^{p}\int_{\mathcal{C}} \mathrm{d}m(\lambda_j)\,F^+_{\ell_j}(\lambda_j)\right]\left[\prod_{j=p+1}^{m}\int_{\mathcal{C}} \mathrm{d}\overline{m}(\lambda_j)\,F^-_{\ell_j}(\lambda_j)\right] \frac{\det_{j,k=1,\dots,m}\left[-G(\lambda_j,\nu_k)\right]}{\prod_{1\le j<k\le m}\mathrm{sh}(\lambda_j-\lambda_k-\eta)\,\mathrm{sh}(\nu_k-\nu_j)}, \quad (29)$$

where we have used the notation

$$\mathrm{d}m(\lambda) = \frac{\mathrm{d}\lambda}{2\pi\mathrm{i}\,\rho(\zeta)(1+\mathfrak{a}(\lambda,\kappa))}, \quad \mathrm{d}\overline{m}(\lambda) = \mathfrak{a}(\lambda,\kappa)\mathrm{d}m(\lambda), \quad (30)$$

$$F^\pm_{\ell_j}(\lambda) = \prod_{k=1}^{\ell_j-1}\mathrm{sh}(\lambda-\nu_k)\prod_{k=\ell_j+1}^{m}\mathrm{sh}(\lambda-\nu_k\mp\eta), \quad \ell_j = \begin{cases}\varepsilon_j^+ & j=1,\dots,p\\ \varepsilon^-_{m-j+1} & j=p+1,\dots,m\end{cases}$$

with ε_j^+ the jth plus in the sequence $(\varepsilon_j)_{j=1}^m$, ε_j^- the jth minus sign in the sequence $(\varepsilon'_j)_{j=1}^m$ and p the number of plus signs in $(\varepsilon_j)_{j=1}^m$. The function G is new here. It is defined as the solution of the linear integral equation

$$G(\lambda,\nu) = q^{-\alpha}\,\mathrm{cth}(\lambda-\nu-\eta) - \rho(\xi)\,\mathrm{cth}(\lambda-\nu) + \int_{\mathcal{C}}\mathrm{d}m(\mu)K_\alpha(\lambda-\mu)G(\mu,\nu), \quad (31)$$

where $\xi = \mathrm{e}^\nu$, and the kernel

$$K_\alpha(\lambda) = q^{-\alpha}\,\mathrm{cth}(\lambda-\eta) - q^\alpha\,\mathrm{cth}(\lambda+\eta) \quad (32)$$

is a deformed version of (24).

Equation (29) is a generalization to finite α of the multiple integral formulae first derived in [11, 15]. To simplify the notation we shall sometimes suppress the dependence of the density matrix elements on κ and α.

4 The case m = 1

For $m = 1$ there are only two non-vanishing density matrix elements. They are related to the function ρ by the reduction relations (19) which imply that

$$\begin{pmatrix} D_+^+(\xi)\\ D_-^-(\xi)\end{pmatrix} = \frac{1}{q^\alpha - q^{-\alpha}}\begin{pmatrix}-q^{-\alpha} & 1\\ q^\alpha & -1\end{pmatrix}\begin{pmatrix}1\\ \rho(\xi)\end{pmatrix}. \quad (33)$$

When we insert equation (29) for $m = 1$ here, we do not obtain an independent equation, but rather an interesting identity for ρ (recall that ρ appears in the measure),

$$\rho(\xi) = q^{-\alpha} - (q^{\alpha} - q^{-\alpha}) \int_{\mathcal{C}} \mathrm{d}m(\mu) G(\mu, \nu) \,. \tag{34}$$

It allows us to calculate the asymptotic behaviour of the function G,

$$\lim_{\mathrm{Re}\lambda \to \pm\infty} G(\lambda, \nu) = 0 \,. \tag{35}$$

5 Factorization of the density matrix for m = 2

The factorization of the multiple integrals for the ground state density matrix was discovered in [10]. In that case the integrand consists of explicit functions whose analytic properties were used in the calculation. In the finite temperature case a different factorization technique had to be invented. As was demonstrated in [3] the linear integral equation for the function G, appropriately used under the multiple integral, can be viewed as the source of the factorization, at least for the special case of the isotropic chain at $\alpha = 0$. For the XXZ chain outside the isotropic point and without the disorder parameter α, however, that trick does not work anymore. Here we shall see that a finite α allows us to perform the factorization of the density matrix in much the same way as in [3].

Let us consider $m = 2$ in (29). There are six non-vanishing matrix elements in this case, one for $p = 0$, four for $p = 1$ and one for $p = 2$. We shall concentrate on the case $p = 1$, since the matrix elements for $p = 0$ or 2 can be obtained from those for $p = 1$ by means of the reduction relation (19). After substituting $w_j = \mathrm{e}^{2\mu_j}$ and $\xi_j = \mathrm{e}^{\nu_j}$, $j = 1, 2$, the corresponding integrals are all of the form

$$\mathcal{I} = \frac{1}{\xi_2^2 - \xi_1^2} \int_{\mathcal{C}} \mathrm{d}m(\mu_1) \int_{\mathcal{C}} \mathrm{d}\overline{m}(\mu_2) \det\bigl[G(\mu_j, \nu_k)\bigr] r(w_1, w_2) \,, \tag{36}$$

where

$$r(w_1, w_2) = \frac{p(w_1, w_2)}{w_1 - q^2 w_2} \,, \quad p(w_1, w_2) = c_0 w_1 w_2 + c_1 w_1 + c_2 w_2 + c_3 \,. \tag{37}$$

The coefficients c_j are different for the four different matrix elements. They are listed in table 1.

Inserting

$$\mathrm{d}\overline{m}(\mu) = \frac{\mathrm{d}\lambda}{2\pi \mathrm{i} \rho(\mathrm{e}^{\mu})} - \mathrm{d}m(\mu) \tag{38}$$

into (36) and taking into account that $\rho(\mathrm{e}^{\mu})$ is analytic and non-zero inside $\mathcal{C}$ we obtain

$$\begin{aligned} \mathcal{I}(\xi_2^2 - \xi_1^2) = & - \int_{\mathcal{C}} \mathrm{d}m(\mu) \det \begin{pmatrix} G(\mu, \nu_1) & G(\mu, \nu_2) \\ r(w, \xi_1^2) & r(w, \xi_2^2) \end{pmatrix} \\ & - \int_{\mathcal{C}} \mathrm{d}m(\mu_1) \int_{\mathcal{C}} \mathrm{d}m(\mu_2) \det\bigl[G(\mu_j, \nu_k)\bigr] r(w_1, w_2) \,, \end{aligned} \tag{39}$$

$\begin{smallmatrix}\varepsilon_1' & \varepsilon_2' \\ \varepsilon_1 & \varepsilon_2\end{smallmatrix}$	c_0	c_1	c_2	c_3
$\begin{smallmatrix}+ & - \\ + & -\end{smallmatrix}$	1	$-\xi_1^2$	$-q^2\xi_2^2$	$q^2\xi_1^2\xi_2^2$
$\begin{smallmatrix}- & + \\ - & +\end{smallmatrix}$	q^2	$-\xi_2^2$	$-q^2\xi_1^2$	$\xi_1^2\xi_2^2$
$\begin{smallmatrix}+ & - \\ - & +\end{smallmatrix}$	$q\xi_2/\xi_1$	$-q\xi_1\xi_2$	$-q\xi_1\xi_2$	$q\xi_1^3\xi_2$
$\begin{smallmatrix}- & + \\ + & -\end{smallmatrix}$	$q\xi_1/\xi_2$	$-q^{-1}\xi_1\xi_2$	$-q^3\xi_1\xi_2$	$q\xi_1\xi_2^3$

Table 1: The coefficients of the polynomial p.

where $w = \mathrm{e}^{2\mu}$. Here the first integral is already factorized. Under the second integral the integration measures now appear symmetrically. Hence, we may replace $r(w_1,w_2)$ by $(r(w_1,w_2) - r(w_2,w_1))/2$.

Following [3] we want to use the integral equation (31) under the second integral in (39). This is possible if rational functions $F(w_1,w_2)$ and $g(w)$ exist, such that

$$r(w_1,w_2) - r(w_2,w_1) = F(w_1,w_2) + g(w_1)K_\alpha(\mu_1-\mu_2) - g(w_2)K_\alpha(\mu_2-\mu_1)\,, \tag{40}$$

and the antisymmetric function $F(w_1,w_2)$ is a sum of factorized functions in w_1 and w_2. Then F considered as a function of w_1 cannot have poles whose position depends on w_2. In particular, the residue at $w_1 = q^2 w_2$ must vanish. Using this in (40) with the explicit forms of r and K_α inserted we obtain a difference equation for g,

$$g(q^2w)y^{-1} - g(w)y = \frac{p(q^2w,w)}{2q^2w}\,. \tag{41}$$

Here $y = q^\alpha$. Clearly this equation has a solution of the form

$$g(w) = g_+ w + g_0 + \frac{g_-}{w}\,. \tag{42}$$

The coefficients are easily obtained by substituting the latter expression into (41),

$$g_+ = \frac{c_0 y}{2(q^2-y^2)}\,, \quad g_- = \frac{c_3 y}{2(1-q^2y^2)}\,, \quad g_0 = \frac{(c_1+q^{-2}c_2)y}{2(1-y^2)}\,. \tag{43}$$

Substituting g back into (40) we obtain $F(w_1,w_2) = f(w_1) - f(w_2)$, where

$$f(w) = (y-y^{-1})\Big(g_+w - \frac{g_-}{w}\Big)\,. \tag{44}$$

Consequentially

$$r(w_1,w_2) = f(w_1) + g(w_1)K_\alpha(\mu_1-\mu_2) + \text{symmetric function.} \tag{45}$$

With this we can factorize the second integral in (39) by means of the integral

equation (31),

$$
\begin{aligned}
\int_{\mathcal{C}} \mathrm{d}m(\mu_1) \int_{\mathcal{C}} \mathrm{d}m(\mu_2) \det\bigl[G(\mu_j,\nu_k)\bigr] r(w_1,w_2) \\
= (y-y^{-1}) \det \begin{pmatrix} g_+\varphi_+(\nu_1) - g_-\varphi_-(\nu_1) & g_+\varphi_+(\nu_2) - g_-\varphi_-(\nu_2) \\ \varphi_0(\nu_1) & \varphi_0(\nu_2) \end{pmatrix} \\
+ \int_{\mathcal{C}} \mathrm{d}m(\mu) \det \begin{pmatrix} G(\mu,\nu_1) & G(\mu,\nu_2) \\ g(w)H(\mu,\nu_1;y^{-1}) & g(w)H(\mu,\nu_2;y^{-1}) \end{pmatrix}, \quad (46)
\end{aligned}
$$

where

$$
\varphi_j(\nu) = \int_{\mathcal{C}} \mathrm{d}m(\mu)\, w^j G(\mu,\nu), \quad j = +,0,-, \tag{47a}
$$

$$
H(\mu,\nu;y^{-1}) = \rho(\xi)\operatorname{cth}(\mu-\nu) - y^{-1}\operatorname{cth}(\mu-\nu-\eta). \tag{47b}
$$

Finally we substitute (46) into (39) and further simplify the resulting expression using the identities

$$
\begin{aligned}
g(w)H(\mu,\nu;y^{-1}) = g(\xi^2)H(\mu,\nu;y) - \frac{p(q^2\xi^2,\xi^2)}{2q^2\xi^2}\operatorname{cth}(\mu-\nu-\eta) \\
- \varphi_0(\nu)\bigl(f(w) - f(\xi^2)\bigr) + \frac{y^{-1}}{y-y^{-1}}\bigl(f(\xi^2) - f(q^2\xi^2)\bigr), \quad (48a)
\end{aligned}
$$

$$
r(w,\xi^2) = \frac{p(q^2\xi^2,\xi^2)}{2q^2\xi^2}\operatorname{cth}(\mu-\nu-\eta) - \frac{p(-q^2\xi^2,\xi^2)}{2q^2\xi^2}. \tag{48b}
$$

Then

$$
\begin{aligned}
\mathcal{I} = \frac{g(\xi_2^2)\Psi(\xi_2,\xi_1) - g(\xi_1^2)\Psi(\xi_1,\xi_2)}{\xi_2^2-\xi_1^2} + \frac{(c_1 - q^{-2}c_2)(\rho(\xi_1)-\rho(\xi_2))}{2(\xi_2^2-\xi_1^2)(y-y^{-1})} \\
+ \frac{(y^{-1}-\rho(\xi_1))(y-\rho(\xi_2))\,f(\xi_2^2) - (y^{-1}-\rho(\xi_2))(y-\rho(\xi_1))\,f(\xi_1^2)}{(\xi_2^2-\xi_1^2)(y-y^{-1})^2}, \quad (49)
\end{aligned}
$$

where

$$
\Psi(\xi_1,\xi_2) = \int_{\mathcal{C}} \mathrm{d}m(\mu) G(\mu,\nu_2)\bigl(q^\alpha \operatorname{cth}(\mu-\nu_1-\eta) - \rho(\xi_1)\operatorname{cth}(\mu-\nu_1)\bigr). \tag{50}
$$

Equation (49) determines the four density matrix elements for $p=1$ in factorized form. Note that the matrix elements depend on only two transcendental functions ρ and Ψ. The remaining two non-zero density matrix elements for $m=2$ follow from (49) by means of the reduction relations (19),

$$
D^{++}_{++}(\xi_1,\xi_2) = \frac{\rho(\xi_1) - y^{-1}}{y-y^{-1}} - D^{+-}_{+-}(\xi_1,\xi_2), \tag{51a}
$$

$$
D^{--}_{--}(\xi_1,\xi_2) = \frac{y-\rho(\xi_1)}{y-y^{-1}} - D^{-+}_{-+}(\xi_1,\xi_2). \tag{51b}
$$

We shall give a fully explicit matrix representation of the factorized density matrix for $m=2$ below, after we have introduced the function ω.

6 The function ω

In the recent work [19] is was shown that the correlation functions defined by the inhomogeneous and α-twisted density matrix (16) factorize and can all be expressed in terms of only two transcendental functions, the function ρ entering the reduction relations (19) and another function ω which in [19] was defined as the expectation value of a product of two creation operators and was represented by a determinant formula. The approach of [19] is slightly different from ours here in that the lattice used in [19] is homogeneous in 'horizontal direction' (all the ξs in (16) are taken to be 1 from the outset). For the ground state both cases lead to the same function ω (see section 5.3 and 5.4 of [9]). In particular, in the inhomogeneous case, following sections 5.1 and 5.3 of [9], we have[‡]

$$\omega(\xi_1,\xi_2) = -\big\langle \mathbf{c}^*_{[1,2]}(\xi_2,\alpha)\mathbf{b}^*_{[1,2]}(\xi_1,\alpha-1)(1)\big\rangle \,. \tag{52}$$

Replacing the vacuum expectation value by the expectation value calculated with the density matrix (16) we take (52) as our definition of the function ω. In our case ω depends on two twist parameters κ and α. We indicate this by writing $\omega(\xi_1,\xi_2|\kappa,\alpha)$. The construction of the operators $\mathbf{b}^*_{[1,2]}$ and $\mathbf{c}^*_{[1,2]}$ is explained in [9]. For the product needed in (52) we find the explicit expression

$$\begin{aligned}
&\xi^{-\alpha}\mathbf{c}^*_{[1,2]}(\xi_2,\alpha)\mathbf{b}^*_{[1,2]}(\xi_1,\alpha-1)(1) = \\
&\qquad \left(\frac{q^{\alpha-1}\xi^{-1}}{q\xi-q^{-1}\xi^{-1}} - \frac{q^{1-\alpha}\xi^{-1}}{q^{-1}\xi-q\xi^{-1}} + \frac{q^\alpha-q^{-\alpha}}{2}\right)\sigma^z\otimes\sigma^z \\
&\qquad + \frac{q^\alpha-q^{-\alpha}}{2}\left(\frac{q^{-1}\xi^{-1}}{q\xi-q^{-1}\xi^{-1}} - \frac{q\xi^{-1}}{q^{-1}\xi-q\xi^{-1}}\right)\big(I_2\otimes\sigma^z - \sigma^z\otimes I_2\big) \\
&\qquad + 2\left(\frac{q^\alpha}{q\xi-q^{-1}\xi^{-1}} - \frac{q^{-\alpha}}{q^{-1}\xi-q\xi^{-1}}\right)\big(\sigma^+\otimes\sigma^- + \sigma^-\otimes\sigma^+\big) \\
&\qquad + (q^\alpha-q^{-\alpha})\left(\frac{1}{q\xi-q^{-1}\xi^{-1}} + \frac{1}{q^{-1}\xi-q\xi^{-1}}\right)\big(\sigma^+\otimes\sigma^- - \sigma^-\otimes\sigma^+\big)\,,
\end{aligned} \tag{53}$$

where $\xi=\xi_1/\xi_2$. Inserting this into (52) and calculating the average with the factorized two-site density matrix of the previous section we obtain

$$\omega(\xi_1,\xi_2|\kappa,\alpha) = 2\xi^\alpha\Psi(\xi_1,\xi_2) - \Delta\psi(\xi) + 2\big(\rho(\xi_1)-\rho(\xi_2)\big)\psi(\xi)\,. \tag{54}$$

Here we adopted the notation from [9],

$$\psi(\xi) = \frac{\xi^\alpha(\xi^2+1)}{2(\xi^2-1)}\,, \tag{55}$$

and Δ is the difference operator whose action on a function f is defined by $\Delta f(\xi) = f(q\xi)-f(q^{-1}\xi)$.

[‡]More precisely this function was denoted $(\omega_0-\omega)(\xi_1/\xi_2,\alpha)$ in [9].

The remaining part of this section is devoted to the exploration of the properties of ω. First of all we substitute ω back into the equation for the two-site density matrix, which can then be expressed entirely in terms of ω and a function

$$\varphi(\zeta|\kappa,\alpha) = \frac{\mathrm{ch}(\alpha\eta) - \rho(\zeta)}{\mathrm{sh}(\alpha\eta)} \tag{56}$$

which is sometimes more convenient than the function ρ itself. We obtain

$$\begin{aligned}
D_N(\xi_1,\xi_2|\kappa,\alpha) = {} & \frac{1}{4} I_2 \otimes I_2 \\
& - \frac{1}{4(q^{\alpha-1} - q^{1-\alpha})}\left(\frac{\xi^{1-\alpha}\omega_{12} - \xi^{\alpha-1}\omega_{21}}{\xi - \xi^{-1}} + \frac{\varphi_1\varphi_2(q^\alpha - q^{-\alpha})}{2}\right) \\
& \left(\frac{q-q^{-1}}{2} I_2 \otimes \sigma^z - \frac{q+q^{-1}}{2}\sigma^z \otimes \sigma^z + \xi^{-1}\sigma^+ \otimes \sigma^- + \xi\sigma^- \otimes \sigma^+\right) \\
& - \frac{1}{4(q^{\alpha+1} - q^{-\alpha-1})}\left(\frac{\xi^{-\alpha-1}\omega_{12} - \xi^{\alpha+1}\omega_{21}}{\xi - \xi^{-1}} + \frac{\varphi_1\varphi_2(q^\alpha - q^{-\alpha})}{2}\right) \\
& \left(-\frac{q-q^{-1}}{2} I_2 \otimes \sigma^z - \frac{q+q^{-1}}{2}\sigma^z \otimes \sigma^z + \xi\sigma^+ \otimes \sigma^- + \xi^{-1}\sigma^- \otimes \sigma^+\right) \\
& - \frac{\xi^{-\alpha}\omega_{12} - \xi^{\alpha}\omega_{21}}{4(\xi - \xi^{-1})(q^\alpha - q^{-\alpha})}\big((\xi + \xi^{-1})\sigma^z \otimes \sigma^z - (q + q^{-1})(\sigma^+ \otimes \sigma^- + \sigma^- \otimes \sigma^+)\big) \\
& - \frac{1}{4}\big(\varphi_1 \sigma^z \otimes I_2 + \varphi_2 I_2 \otimes \sigma^z\big) - \frac{q-q^{-1}}{4(\xi - \xi^{-1})}(\varphi_1 - \varphi_2)(\sigma^+ \otimes \sigma^- - \sigma^- \otimes \sigma^+)\,,
\end{aligned} \tag{57}$$

where we introduced the abbreviations $\omega_{jk} = \omega(\xi_j,\xi_k|\kappa,\alpha)$ and $\varphi_j = \varphi(\xi_j|\kappa,\alpha)$.

For the limit $\alpha \to 0$ the properties of the functions φ and ω with respect to negating κ and α are important. They follow from the fact that the R-matrix is invariant under spin reversal,

$$R(\lambda) = (\sigma^x \otimes \sigma^x) R(\lambda) (\sigma^x \otimes \sigma^x)\,. \tag{58}$$

Introducing the spin reversal operator $J = \sigma_1^x \dots \sigma_N^x$ we conclude with (58) that

$$T_a(\zeta,-\kappa) = \sigma_a^x J\, T_a(\zeta,\kappa)\, J \sigma_a^x\,. \tag{59}$$

It follows that $t(\zeta,-\kappa) = Jt(\zeta,\kappa)J$. Hence,

$$J|\kappa\rangle = |-\kappa\rangle\,, \tag{60a}$$

$$\Lambda(\zeta,\kappa) = \Lambda(\zeta,-\kappa)\,. \tag{60b}$$

The latter two equations used in the definition (16) of the α-twisted density matrix imply that

$$D_N(\xi_1,\dots,\xi_m|-\kappa,-\alpha) = (\sigma^x)^{\otimes m} D_N(\xi_1,\dots,\xi_m|\kappa,\alpha)\,(\sigma^x)^{\otimes m}\,. \tag{61}$$

From (20), (60b) we obtain the relation

$$\varphi(\zeta|-\kappa,-\alpha) = -\varphi(\zeta|\kappa,\alpha)\,. \tag{62}$$

Equation (61) together with (52)-(54) and the expressions for the density matrix elements of the previous section implies that

$$\omega(\xi_1,\xi_2|\kappa,\alpha)=\omega(\xi_2,\xi_1|-\kappa,-\alpha)\,. \tag{63}$$

Our next step is to verify that the function ω given by the formula (54) satisfies a property called the 'normalization condition' by the authors of [19] (see equation (6.10) there). So we come back to the case of finite Trotter number N with arbitrary inhomogeneity parameters $\beta_j,\ j=1,\dots,N$ as it is written in (5). We shall also use multiplicative parameters $\tau_j=e^{\beta_j}$.

We consider the normalization condition in the following form

$$\begin{aligned}\big(\omega(\zeta,\xi|\kappa,\alpha)+\overline{D}_\zeta\overline{D}_\xi\Delta_\zeta^{-1}\psi(\zeta/\xi)\big)\big|_{\zeta=\tau_j}+&\\ +\rho(\tau_j)\big(\omega(\zeta,\xi|\kappa,\alpha)+\overline{D}_\zeta\overline{D}_\xi\Delta_\zeta^{-1}\psi(\zeta/\xi)\big)\big|_{\zeta=q^{-1}\tau_j}&=0\,,\end{aligned} \tag{64}$$

$j=1,\dots N$, which can be obtained from the integral in (6.10) of [19] by taking the residues and using the TQ-relation (4.2) of that paper. Also let us recall the definition

$$\overline{D}_\zeta g(\zeta)=g(q\zeta)+g(q^{-1}\zeta)-2\rho(\zeta)g(\zeta)\,. \tag{65}$$

Actually, (6.10) of [19] comprises one more equation related to the residue at $\zeta^2=0$. This case needs separate treatment and will be discussed below.

First we use the following difference equation for the function Ψ defined by (50),

$$\begin{aligned}\Psi(\xi_1,\xi_2)+\rho(\xi_1)q^{-\alpha}\Psi(q^{-1}\xi_1,\xi_2)&=\frac{G(\nu_1,\nu_2)}{1+\overline{\mathfrak{a}}(\nu_1,\kappa)}-\rho(\xi_1)q^{-\alpha}\frac{G(\nu_1-\eta,\nu_2)}{1+\mathfrak{a}(\nu_1-\eta,\kappa)}\\ &+\rho(\xi_2)\,\mathrm{cth}(\nu_1-\nu_2)-q^{-\alpha}\,\mathrm{cth}(\nu_1-\nu_2-\eta)\\ &-q^{-\alpha}\big(\rho(\xi_1)\rho(q^{-1}\xi_1)-1\big)\int_{\mathcal{C}}\mathrm{d}m(\mu)G(\mu,\nu_2)\,\mathrm{cth}(\mu-\nu_1+\eta)\,,\end{aligned} \tag{66}$$

where $\overline{\mathfrak{a}}=1/\mathfrak{a}$ by definition. This equation is the result of an analytical continuation defined for $\Psi(q^{-1}\xi_1,\xi_2)$ through an appropriate deformation of the integration contour in (50). Some simplifications occur in the limit $\nu_1\to\beta_j$ or equivalently $\xi_1\to\tau_j$, namely, since $\mathfrak{a}(\beta_j,\kappa)=\overline{\mathfrak{a}}(\beta_j-\eta,\kappa)=0$ or $\overline{\mathfrak{a}}(\beta_j,\kappa)=\mathfrak{a}(\beta_j-\eta,\kappa)=\infty$, the first two terms in the right hand side of (66) do not contribute. Then we have

$$\rho(\tau_j)\rho(q^{-1}\tau_j)=\frac{Q^-(q^{-1}\tau_j;\kappa+\alpha)Q^+(\tau_j;\kappa)}{Q^-(\tau_j;\kappa+\alpha)Q^+(q^{-1}\tau_j;\kappa)}\cdot\frac{Q^-(\tau_j;\kappa+\alpha)Q^+(q^{-1}\tau_j;\kappa)}{Q^-(q^{-1}\tau_j;\kappa+\alpha)Q^+(\tau_j;\kappa)}=1$$

with the Q-functions $Q^\pm$ defined in [19]. This means that also the last term in the right hand side of (66) does not contribute. Hence, we obtain

$$\Psi(\tau_j,\xi_2)+\rho(\tau_j)q^{-\alpha}\Psi(q^{-1}\tau_j,\xi_2)=\rho(\xi_2)\,\mathrm{cth}(\beta_j-\nu_2)-q^{-\alpha}\,\mathrm{cth}(\beta_j-\nu_2-\eta)\,. \tag{67}$$

Note that the right hand side is, up to the sign, equal to the driving term in the integral equation (31) for G.

If we take the formula (54) and use (67) then, after some algebra, we obtain

$$\begin{aligned}
&\omega(\tau_j,\xi_2|\kappa,\alpha)+\rho(\tau_j)\omega(q^{-1}\tau_j,\xi_2|\kappa,\alpha)=\\
&\quad-\big(\Delta_\zeta\psi(\zeta/\xi_2)\big)\big|_{\zeta=\tau_j}-\rho(\tau_j)\big(\Delta_\zeta\psi(\zeta/\xi_2)\big)\big|_{\zeta=q^{-1}\tau_j}\\
&\quad+2(\rho(\tau_j)+\rho(\xi_2))\,\psi(\tau_j/\xi_2)-2(1+\rho(\tau_j)\rho(\xi_2))\,\psi(q^{-1}\tau_j/\xi_2)\,.
\end{aligned}\tag{68}$$

Now we need to check that this equation is equivalent to (64). To this end we should verify the following equality

$$\begin{aligned}
&\big(\overline{D}_\zeta\overline{D}_\xi\Delta_\zeta^{-1}\psi(\zeta/\xi)\big)\big|_{\zeta=\tau_j}+\rho(\tau_j)\big(\overline{D}_\zeta\overline{D}_\xi\Delta_\zeta^{-1}\psi(\zeta/\xi)\big)\big|_{\zeta=q^{-1}\tau_j}=\\
&\qquad\big(\Delta_\zeta\psi(\zeta/\xi_2)\big)\big|_{\zeta=\tau_j}+\rho(\tau_j)\big(\Delta_\zeta\psi(\zeta/\xi_2)\big)\big|_{\zeta=q^{-1}\tau_j}\\
&\qquad-2(\rho(\tau_j)+\rho(\xi_2))\psi(\tau_j/\xi_2)+2(1+\rho(\tau_j)\rho(\xi_2))\psi(q^{-1}\tau_j/\xi_2)\,.
\end{aligned}\tag{69}$$

Using the definition (65) we come after a little algebra to the following expression for an arbitrary function $g(\zeta)$

$$\begin{aligned}
\overline{D}_\zeta\overline{D}_\xi\,g(\zeta/\xi)&=\Delta_\zeta^2\,g(\zeta/\xi)+4(1-\rho(\zeta))\,(1-\rho(\xi))\,g(\zeta/\xi)\\
&\quad-2(\rho(\zeta)+\rho(\xi))\,(g(q\zeta/\xi)+g(q^{-1}\zeta/\xi)-2g(\zeta/\xi))\,.
\end{aligned}\tag{70}$$

Now take

$$\begin{aligned}
&\big(\overline{D}_\zeta\overline{D}_\xi\,g(\zeta/\xi)\big)\big|_{\zeta=\tau_j}+\rho(\tau_j)\big(\overline{D}_\zeta\overline{D}_\xi\,g(\zeta/\xi)\big)\big|_{\zeta=q^{-1}\tau_j}=\\
&\quad\big(\Delta_\zeta^2\,g(\zeta/\xi)\big)\big|_{\zeta=\tau_j}+\big(\Delta_\zeta^2\,g(\zeta/\xi)\big)\big|_{\zeta=q^{-1}\tau_j}-2(\rho(\tau_j)+\rho(\xi))\big(\Delta_\zeta\,g(\zeta/\xi)\big)\big|_{\zeta=\tau_j}\\
&\quad+2(1+\rho(\tau_j)\rho(\xi))\big(\Delta_\zeta\,g(\zeta/\xi)\big)\big|_{\zeta=q^{-1}\tau_j}\,.
\end{aligned}\tag{71}$$

If we substitute $g(\zeta/\xi)=\Delta_\zeta^{-1}\psi(\zeta/\xi)$ and take $\xi=\xi_2$, then we immediately arrive at the equality (69).

As was mentioned above, there is one more case to be considered, corresponding to the contour Γ_0, i.e. to the residue at $\zeta^2=0$ in equation (6.10) of [19] which has to vanish. Its vanishing follows from

$$\begin{aligned}
&\lim_{\xi_1\to 0}\xi^{-\alpha}\big(\omega(\xi_1,\xi_2)+\overline{D}_{\xi_1}\overline{D}_{\xi_2}\Delta_{\xi_1}^{-1}\psi(\xi)\big)=\\
&\qquad\frac{2q^{-\kappa}}{q^{\kappa}+q^{-\kappa}}\left[\rho(\xi_2)-q^{-\alpha}+(q^{\alpha}-q^{-\alpha})\int_{\mathcal{C}}\mathrm{d}m(\mu)G(\mu,\nu_2)\right]=0\,.
\end{aligned}\tag{72}$$

Here we have used (50), (54), (55), (70) as well as the fact that $\lim_{\nu\to-\infty}\rho(\xi)=(q^{\alpha+\kappa}+q^{-\alpha-\kappa})/(q^{\kappa}+q^{-\kappa})$ in the first equation and the identity (34) in the second equation.

The normalization condition just shown to be satisfied by our function ω defined in (52) is the main ingredient in our proof that ω is in fact the same function as introduced in equation (7.2) of [19]. Let us consider ω as a function of ξ_1. As was shown in [19]

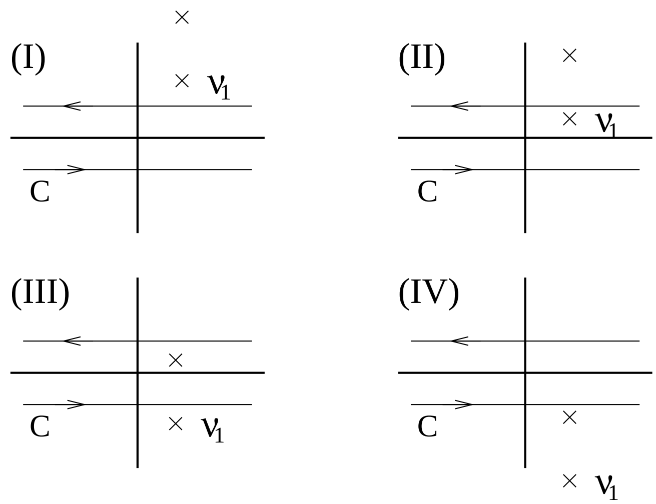

Figure 2: Four cases to be considered for the analytic continuation of $\Psi(\xi_1,\xi_2)$ with respect to ν_1. Here $\mathcal{C}$ is the canonical contour of figure 1.

the function $\rho(\xi_1)$ depends only on ξ_1^2. The same is then true for $\Psi(\xi_1,\xi_2)$ from (50). Using (54) we conclude that $\xi^{-\alpha}\omega(\xi_1,\xi_2|\kappa,\alpha)$ is a function of ξ_1^2. From its definition (52) and from (16), (53) we see that ω is rational in ξ_1^2 of the form $P(\xi_1^2)/Q(\xi_1^2)$, where P and Q are polynomials. Clearly both of them are at most of degree $N+2$. The zeros of Q are the N zeros of the transfer matrix eigenvalue $\Lambda(\xi_1,\kappa)$ plus two zeros at $q^{\pm 2}\xi_2^2$ stemming from the two simple poles of $\xi^{-\alpha}\mathbf{c}^*_{[1,2]}(\xi_2,\alpha)\mathbf{b}^*_{[1,2]}(\xi_1,\alpha-1)(1)$. Comparing now with the definition (7.2) of [19] we see that the functions there has precisely the same structure. It is rational of the form $\widetilde{P}(\xi_1^2)/\widetilde{Q}(\xi_1^2)$ with two polynomials $\widetilde{P}$, $\widetilde{Q}$ at most of degree $N+2$. Q and $\widetilde{Q}$ have the same zeros. We may therefore assume that they are identical. In order to show that P and $\widetilde{P}$ also agree we have to provide $N+3$ relations. $N+1$ of them are given by the normalization condition above. Another two come from the residues at the two trivial poles.

Since they are outside the canonical contour, we have to consider again the analytic continuation of the integral (50) defining Ψ with respect to ξ_1. There are four regions depending on the location of ν_1 relative to the contour (see figure 2). Using (50) we obtain

$$\Psi(\xi_1,\xi_2) = \int_{\mathcal{C}} \mathrm{d}m(\mu) G(\mu,\nu_2)\big(q^\alpha \operatorname{cth}(\mu-\nu_1-\eta) - \rho(\xi_1)\operatorname{cth}(\mu-\nu_1)\big)$$
$$- \begin{cases} \dfrac{G(\nu_1,\nu_2)}{1+\mathfrak{a}(\nu_1,\kappa)} & \text{case (I)} \\ 0 & \text{case (II)} \\ \dfrac{G(\nu_1,\nu_2)}{1+\mathfrak{a}(\nu_1,\kappa)} + \dfrac{q^\alpha G(\nu_1+\eta,\nu_2)}{(1+\mathfrak{a}(\nu_1+\eta,\kappa))\rho(q\xi_1)} & \text{case (III)} \\ \dfrac{G(\nu_1,\nu_2)}{1+\mathfrak{a}(\nu_1,\kappa)} & \text{case (IV)}\,. \end{cases} \tag{73}$$

Then, e.g. be means of the integral equation (31)

$$\operatorname{res}_{\xi_1^2=q^2\xi_2^2}\Psi(\xi_1,\xi_2) = \\ -\frac{2\xi_2^2 q^{2-\alpha}}{(1+\mathfrak{a}(\nu_2+\eta,\kappa))(1+\overline{\mathfrak{a}}(\nu_2,\kappa))} = -\frac{2\xi_2^2 q^{2-\alpha} a(\xi_2 q) d(\xi_2)}{\Lambda(\xi_2 q,\kappa)\Lambda(\xi_2,\kappa)}\,, \tag{74a}$$

$$\operatorname{res}_{\xi_1^2=q^{-2}\xi_2^2}\Psi(\xi_1,\xi_2) = \\ \frac{2\xi_2^2 q^{\alpha-2}}{(1+\mathfrak{a}(\nu_2,\kappa))(1+\overline{\mathfrak{a}}(\nu_2-\eta,\kappa))} = \frac{2\xi_2^2 q^{\alpha-2} a(\xi_2) d(\xi_2 q^{-1})}{\Lambda(\xi_2,\kappa)\Lambda(\xi_2 q^{-1},\kappa)}\,, \tag{74b}$$

where a and d are the vacuum expectation values of the diagonal elements of $T(\zeta)$. Since the ratios on the right hand side are invariant under changing the normalization of the R-matrix, we can directly compare the residues obtained from (54), (74) with those obtained from equation (7.2) of [19]. We find agreement, which completes the proof.

What if we consider (54) as the definition of ω? Then, in addition, we have to show that there are no poles other than the two trivial ones and those at the location of the zeros of $\Lambda(\xi_1,\kappa)$. But this is immediately clear from (73). The integral has only poles at the zeros of $\Lambda(\xi_1,\kappa)$. In case (I) there is one additional pole at $\nu_1=\nu_2+\eta$ with residue (74a). The simple poles of $G(\nu_1,\nu_2)$ at $\lambda_j+\eta$, where the λ_j are the Bethe roots (see appendix A), are canceled by the simple poles of $\mathfrak{a}(\nu_1,\kappa)$ (see equation (A.6a)). In cases (II) and (IV) there is nothing to show. In case (III) we have one additional pole at $\nu_1=\nu_2-\eta$ with residue (74b). The simple poles at $\lambda_j-\eta$ have vanishing residue due to (A.6a) and since

$$\operatorname{res}_{\nu_1=\lambda_j-\eta} G(\nu_1,\nu_2) = -\frac{q^\alpha G(\lambda_j,\nu_2)}{\rho(\zeta_j)\mathfrak{a}'(\lambda_j)}\,. \tag{75}$$

7 The exponential form – preliminary remarks

The main result of [19] is the formula (1.12). It makes the calculation of arbitrary correlation functions possible, because the operators $\mathbf{t}^*,\mathbf{b}^*,\mathbf{c}^*$ generate a basis of the space of quasi-local operators [5]. Although this formula proves the factorization of the correlation functions and allows, in principle, also for their direct numerical evaluation, it may be sometimes preferable to avoid the creation operators and to have an explicit formula for the correlation functions in the standard basis generated by the local operators $e_{j\,\varepsilon}^{\;\varepsilon'}$. We believe that some form of the exponential formula discussed in the previous papers [2–4, 9] must be valid in case of temperature, disorder and magnetic fields as well. Unfortunately, the problem of constructing all operators that appear in this formula remains still open. We hope to come back to it in a future publication. Here we formulate the general properties we expect for these operators and show by examples how they should look like for short distances.

From now on we shall use the notation and the terminology of the paper [9]. In particular we shall be dealing with the space $\mathcal{W}^{(\alpha)}$ of quasi-local operators of the form $q^{2\alpha S(0)}\mathcal{O}$ introduced there. First we define a density operator $D_N^*:\mathcal{W}^{(\alpha)}\to\mathbb{C}$ which

generalizes that one defined by the formulae (33), (34) of [4], namely, for any quasi-local operator $\mathcal{O}$ we define

$$D^*_N(\mathcal{O}) = \langle \mathcal{O} \rangle_{T,\alpha,\kappa} \tag{76}$$

in such a way that

$$D^*_N\bigl(e_1{}^{\varepsilon_1}_{\varepsilon'_1} \dots e_m{}^{\varepsilon_m}_{\varepsilon'_m}\bigr) = D_N{}^{\varepsilon'_1 \dots \varepsilon'_m}_{\varepsilon_1 \dots \varepsilon_m}(\xi_1, \dots, \xi_m | \kappa, \alpha) \tag{77}$$

where D_N is the density matrix defined in (16).

We expect that as before

$$D^*_N(\mathcal{O}) = \mathbf{tr}^\alpha \bigl\{ \exp(\Omega) \bigl(q^{2\alpha S(0)} \mathcal{O} \bigr) \bigr\}, \tag{78}$$

where $\mathbf{tr}^\alpha$ is the α-trace defined in [9] and where the operator Ω consists of two terms like that one constructed in [4]

$$\Omega = \Omega_1 + \Omega_2 \,. \tag{79}$$

In fact, the first term follows from [9, 19]. It must be of the form

$$\Omega_1 = \int \frac{d\zeta_1^2}{2\pi i \zeta_1^2} \int \frac{d\zeta_2^2}{2\pi i \zeta_2^2} \bigl(\omega_0(\zeta_1/\zeta_2|\alpha) - \omega(\zeta_1, \zeta_2|\kappa, \alpha) \bigr) \mathbf{b}(\zeta_1) \mathbf{c}(\zeta_2) \,, \tag{80}$$

where the function ω_0 was defined in [9],

$$\omega_0(\zeta|\alpha) = -\left(\frac{1-q^\alpha}{1+q^\alpha} \right)^2 \Delta_\zeta \psi(\zeta) \,. \tag{81}$$

The second part in the right hand side of (79) should be of the form

$$\Omega_2 = \int \frac{d\zeta^2}{2\pi i \zeta^2} \log(\rho(\zeta)) \mathbf{t}(\zeta) \tag{82}$$

where the operator $\mathbf{t}$ is yet to be determined. In some sense it must be the conjugate of the operator $\mathbf{t}^*$. The integration contour for both, Ω_1 and Ω_2, is taken around all simple poles $\zeta_1, \zeta_2, \zeta = \xi_j$ with $j = 1, \dots, m$ in anti-clockwise direction. The number m is the length of locality of the operator $\mathcal{O}$.

Let us list some of the most important expected properties of the operator $\mathbf{t}$. First, we expect that like $\mathbf{t}^*(\zeta)$ the operator $\mathbf{t}(\zeta)$ is block diagonal,

$$\mathbf{t}(\zeta) : \ \ \mathcal{W}_{\alpha,s} \to \mathcal{W}_{\alpha,s} \,,$$

where, as was explained in [9], $\mathcal{W}_{\alpha,s} \subset \mathcal{W}^{(\alpha)}$ is the space of quasi-local operators of spin s. We will deal below mostly with the sector $s = 0$.

Then we expect $\mathbf{t}(\zeta)$ to have simple poles at $\zeta = \xi_j$. Let us define

$$\mathbf{t}_j = \mathrm{res}_{\zeta=\xi_j} \mathbf{t}(\zeta) \frac{d\zeta^2}{\zeta^2} \tag{83}$$

while

$$\mathbf{t}^*_j = \mathbf{t}^*(\xi_j) \,. \tag{84}$$

In contrast to (83) the operator $\mathbf{t}_j^*$ is well defined only if it acts on the states $X_{[k,l]}$ with $l<j$. This will be always implied below. Let us denote $\mathbf{t}_{[k,l]}(\zeta)$ and respectively $\mathbf{t}_{j[k,l]}$ the operators defined on the interval $[k,l]$ with $k\le j\le l$.

We also expect that R-matrix symmetry holds similar to the formula (2.16) of [9] for $\mathbf{t}^*$,

$$\mathbf{s}_i\,\mathbf{t}_{[k,l]}(\zeta)=\mathbf{t}_{[k,l]}(\zeta)\,\mathbf{s}_i \quad \text{for} \quad k\le i<l\,. \tag{85}$$

Here as was defined in [9]

$$\mathbf{s}_i=K_{i,i+1}\check{\mathbb{R}}_{i,i+1}(\xi_i/\xi_{i+1})\,, \tag{86a}$$

$$\check{\mathbb{R}}_{i,i+1}(\xi_i/\xi_{i+1})(X)=\check{R}_{i,i+1}(\xi_i/\xi_{i+1})X\check{R}_{i,i+1}(\xi_i/\xi_{i+1})^{-1}\,, \tag{86b}$$

$$\check{R}_{i,i+1}(\zeta)=P_{i,i+1}R_{i,i+1}(\zeta)\,, \tag{86c}$$

where $K_{i,j}$ stands for the transposition of arguments ξ_i and ξ_j and $P_{i,j}\in\mathrm{End}(V_i\otimes V_j)$ is the transposition matrix.

The further properties are:

- *Commutation relations*

$$[\mathbf{t}_j,\mathbf{t}_k]_-=[\mathbf{t}_j,\mathbf{b}(\zeta_1)\mathbf{c}(\zeta_2)]_-=0\,. \tag{87}$$

- *Projector property*

$$\mathbf{t}_j^2=\mathbf{t}_j\,. \tag{88}$$

- *Relations with* $\mathbf{t}^*$

$$\begin{aligned}&\mathbf{t}_j\mathbf{t}_k^*=\mathbf{t}_j^*\mathbf{t}_k \quad \text{for} \quad j\neq k\,,\\ &\mathbf{t}_j\mathbf{t}_j^*=\mathbf{t}_j^*, \quad \mathbf{t}_j^*\mathbf{t}_j=0\,.\end{aligned} \tag{89}$$

- *Reduction properties*

$$\mathbf{t}_{1[1,l]}(q^{\alpha\sigma_1^z}X_{[2,l]})=q^{\alpha\sigma_1^z}X_{[2,l]}\,, \tag{90a}$$

$$\mathbf{t}_{j[1,l]}(q^{\alpha\sigma_1^z}X_{[2,l]})=q^{\alpha\sigma_1^z}\mathbf{t}_{j[2,l]}(X_{[2,l]}) \quad \text{for} \quad 1<j\le l\,, \tag{90b}$$

$$\mathbf{t}_{j[1,l]}(X_{[1,l-1]})=\mathbf{t}_{j[1,l-1]}(X_{[1,l-1]}) \quad \text{for} \quad 1\le j<l\,, \tag{90c}$$

$$\mathbf{t}_{l[1,l]}(X_{[1,l-1]})=0\,. \tag{90d}$$

Let us comment on these relations. First of all the commutation relations (87) lead to the factorization of the exponential

$$\exp(\Omega)=\exp(\Omega_1+\Omega_2)=\exp(\Omega_1)\exp(\Omega_2)\,. \tag{91}$$

As we know (see [3, 4, 9] and earlier references therein) the operator Ω_1 becomes nilpotent when it acts on states of finite length. By way of contrast, the operator Ω_2 is not nilpotent, but due to (87) and the projector property (88) one can conclude that

$$\exp(\Omega_2)\big(q^{2\alpha S(0)}X_{[1,l]}\big)=\prod_{j=1}^{l}(1-\mathbf{t}_{j[1,l]}+\rho_j\mathbf{t}_{j[1,l]})\big(X_{[1,l]}\big)q^{2\alpha S(0)}\,, \tag{92}$$

where $\rho_j = \rho(\xi_j)$. The reduction properties (90) look standard except for the first one. It is easy to see that we need all of them in order to have the reduction property (19b) of the density matrix, but still we do not have a good understanding of (90a).

Let us show how the $\mathbf{t}_j$ for $s = 0$ explicitly look like in two particular cases, namely, for $m = 1$ and $m = 2$ where $m = l - k + 1$ and without loss of generality $k = 1$.

$\mathbf{m} = \mathbf{1}$:

$$\mathbf{t}_{1[1,1]} = \frac{q^{\alpha\sigma_1^z} \otimes \sigma_1^z}{q^{\alpha} - q^{-\alpha}} \tag{93}$$

$\mathbf{m} = \mathbf{2}$:

$$\begin{aligned}
\mathbf{t}_{1[1,2]} = & \frac{1}{4}\,\frac{q^{\alpha}+q^{-\alpha}}{q^{\alpha}-q^{-\alpha}} I \otimes \left[\sigma_1^z - \frac{q-q^{-1}}{\xi_1/\xi_2 - \xi_2/\xi_1} \cdot (\sigma_1^+\sigma_2^- - \sigma_1^-\sigma_2^+)\right] + \\
& + \frac{1}{4}\sigma_1^z \otimes \left[\sigma_1^z - \frac{q-q^{-1}}{\xi_1/\xi_2 - \xi_2/\xi_1} \cdot (\sigma_1^+\sigma_2^- - \sigma_1^-\sigma_2^+)\right] + \\
& + \frac{1}{4} q^{\alpha\sigma_1^z}\sigma_2^z \otimes \left[\left(\frac{q^{\sigma_1^z}}{q^{\alpha+1}-q^{-\alpha-1}} + \frac{q^{-\sigma_1^z}}{q^{\alpha-1}-q^{-\alpha+1}}\right)\sigma_1^z\sigma_2^z - \right. \\
& - \frac{(q-q^{-1})(q^{\alpha}+q^{-\alpha})}{2(q^{\alpha+1}-q^{-\alpha-1})(q^{\alpha-1}-q^{-\alpha+1})}(\xi_1/\xi_2 - \xi_2/\xi_1)\cdot(\sigma_1^+\sigma_2^- - \sigma_1^-\sigma_2^+) - \\
& \left. - \frac{(q+q^{-1})(q^{\alpha}-q^{-\alpha})}{2(q^{\alpha+1}-q^{-\alpha-1})(q^{\alpha-1}-q^{-\alpha+1})}(\xi_1/\xi_2 + \xi_2/\xi_1)\cdot(\sigma_1^+\sigma_2^- + \sigma_1^-\sigma_2^+)\right].
\end{aligned} \tag{94}$$

The operator $\mathbf{t}_{2[1,2]}$ can be obtained from $\mathbf{t}_{1[1,2]}$ using the R-matrix symmetry (85),

$$\mathbf{t}_{2[1,2]} = \mathbf{s}_1 \mathbf{t}_{1[1,2]} \mathbf{s}_1^{-1}\,. \tag{95}$$

One can check that all the above properties are fulfilled.

It is interesting to understand how the limit $\alpha \to 0$ works, because, as one can see from (93)-(95), the operators $\mathbf{t}_1$ and $\mathbf{t}_2$ are singular in this limit. More precisely, only the very first term in the expression (94) for $\mathbf{t}_{1[1,2]}$ is singular. In fact, they contribute into the density matrix only in such a combination that this singularity cancels. So, we actually need to calculate the residue with respect to α. In appendix B we will discuss this issue in more detail. We will also show how these operators are related to the 'fermionic' operators $\mathbf{h}_j$ constructed in [2, 4].

8 Conclusions

The main result of this work is the description of the function ω in terms of integrals involving the auxiliary function $\mathfrak{a}$ and the function G, which are solutions of integral equations. As we have experienced in our previous work such type of description is efficient for performing the Trotter limit and for the actual numerical evaluation of correlation functions. We know from [19] that no other functions than ω and ρ are required. Thus, together with [19], we have achieved a rather complete understanding of the mathematical structure of the static correlation functions of the XXZ chain. Our

results are equally valid in the finite temperature as in the finite length case, the only difference being a different driving term in the non-linear integral equation for the auxiliary functions $\mathfrak{a}$.

We expect that our results open a way for further concrete studies of short range correlation functions at finite temperature as initiated in [2–4]. We hope that in the future it will also prove useful in studying field theoretical scaling limits as well as the large distance asymptotics of correlation functions in the XXZ chain.

We have obtained our expression for ω through a novel multiple integral representation of the density matrix of the XXZ chain including a disorder parameter α. We think that this multiple integral representation is also interesting on its own right.

We would like to point out that we obtained a remarkably beautiful and simple characterization of the function Ψ on the inhomogeneous finite lattice through equation (67) and the residua (74). The function Ψ is important because it becomes the transcendental part of ω in the Trotter limit.

We further performed a case study, looking for an operator $\mathbf{t}$, adjoint to $\mathbf{t}^*$ that allows us to write the density matrix in an exponential form even in the presence of a disorder parameter and a finite magnetic field. We obtained explicit expressions for $\mathbf{t}$ for $m = 1, 2$, but so far could not find a general construction behind it. We hope to come back to this latter point in the future.

Acknowledgement. The authors are deeply indebted to M. Jimbo, T. Miwa and F. Smirnov for a fruitful collaboration that led to this paper. They would like to thank A. Klümper, K. Nirov, J. Suzuki, C. Trippe and A. Weiße for helpful and stimulating discussions. Special thanks are due to N. Kitanine for explaining how to derive the multiple integral representation in section 3. This work was financially supported by the Volkswagen Foundation.

Appendix A: Derivation of the multiple integral representation

A multiple integral representation for the density matrix in the non-twisted case $\alpha = 0$ was derived in [13]. Here we shall only indicate which modifications are necessary to include non-zero α and otherwise refer the reader to that work.

First note that

$$\frac{\langle\kappa+\alpha|T^{\varepsilon_1'}_{\varepsilon_1}(\xi_1,\kappa)\dots T^{\varepsilon_m'}_{\varepsilon_m}(\xi_m,\kappa)|\kappa\rangle}{\langle\kappa+\alpha|\prod_{j=1}^m t(\xi_j,\kappa)|\kappa\rangle} = \frac{\langle\kappa|T^{\varepsilon_m}_{\varepsilon_m'}(\xi_m,\kappa)\dots T^{\varepsilon_1}_{\varepsilon_1'}(\xi_1,\kappa)|\kappa+\alpha\rangle}{\langle\kappa|\prod_{j=1}^m t(\xi_j,\kappa)|\kappa+\alpha\rangle}\,, \tag{A.1}$$

because of the symmetry of the R-matrix with respect to transposition. We may therefore start our calculation with

$$\frac{\langle\kappa|T^{\alpha_1}_{\beta_1}(\xi_1,\kappa)\dots T^{\alpha_m}_{\beta_m}(\xi_m,\kappa)|\kappa+\alpha\rangle}{\langle\kappa|\prod_{j=1}^m t(\xi_j,\kappa)|\kappa+\alpha\rangle}\,, \tag{A.2}$$

which brings us closer to the notation of [13].

The left and right eigenvectors $\langle\kappa|$ and $|\kappa+\alpha\rangle$ can be constructed by means of the algebraic Bethe ansatz. They are parameterized by two sets $\{\lambda\} = \{\lambda_j\}_{j=1}^{N/2}$ and

$\{\mu\} = \{\mu_j\}_{j=1}^{N/2}$ of Bethe roots, which are special solutions to the Bethe ansatz equations

$$\frac{q^{-2\kappa}d(\lambda_j)}{a(\lambda_j)}\prod_{k=1}^{N/2}\frac{\mathrm{sh}(\lambda_j-\lambda_k+\eta)}{\mathrm{sh}(\lambda_j-\lambda_k-\eta)} = -1\,, \quad \frac{q^{-2\kappa-2\alpha}d(\mu_j)}{a(\mu_j)}\prod_{k=1}^{N/2}\frac{\mathrm{sh}(\mu_j-\mu_k+\eta)}{\mathrm{sh}(\mu_j-\mu_k-\eta)} = -1 \tag{A.3}$$

for $j = 1,\dots,N/2$. By $a(\lambda)$ and $d(\lambda)$ we denoted here the vacuum expectation values of the diagonal elements of $T(\zeta)$. For its κ-twisted version we shall reserve the notation

$$T(\zeta|\kappa) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda)\end{pmatrix}. \tag{A.4}$$

for the matrix elements. Then the eigenvectors $\langle\kappa|$ and $|\kappa+\alpha\rangle$ are

$$\langle\kappa| = \langle\{\lambda\}| = \langle 0|C(\lambda_1)\dots C(\lambda_{N/2})\,, \tag{A.5a}$$

$$|\kappa+\alpha\rangle = |\{\mu\}\rangle = B(\mu_1)\dots B(\mu_{N/2})|0\rangle\,, \tag{A.5b}$$

where $\langle 0|$ and $|0\rangle$ are the left and right pseudo vacuum states.

With the solutions $\{\lambda\}$ and $\{\mu\}$ of the Bethe ansatz equations we associate the auxiliary functions

$$\mathfrak{a}(\lambda) = \mathfrak{a}(\lambda,\kappa) = \frac{q^{-2\kappa}d(\lambda)}{a(\lambda)}\prod_{k=1}^{N/2}\frac{\mathrm{sh}(\lambda-\lambda_k+\eta)}{\mathrm{sh}(\lambda-\lambda_k-\eta)}\,, \tag{A.6a}$$

$$\mathfrak{a}_\alpha(\lambda) = \mathfrak{a}(\lambda,\kappa+\alpha) = \frac{q^{-2\kappa-2\alpha}d(\lambda)}{a(\lambda)}\prod_{k=1}^{N/2}\frac{\mathrm{sh}(\lambda-\mu_k+\eta)}{\mathrm{sh}(\lambda-\mu_k-\eta)} \tag{A.6b}$$

and the ratio of q-functions

$$\phi(\lambda) = \prod_{j=1}^{N/2}\frac{\mathrm{sh}(\lambda-\mu_j)}{\mathrm{sh}(\lambda-\lambda_j)}\,. \tag{A.7}$$

Then $\langle\{\lambda\}|$ is the 'dominant' left eigenvector of $t(\zeta,\kappa)$ with eigenvalue

$$\Lambda(\zeta,\kappa) = q^\kappa a(\lambda)\left[\prod_{j=1}^{N/2}\frac{\mathrm{sh}(\lambda-\lambda_j-\eta)}{\mathrm{sh}(\lambda-\lambda_j)}\right]\big(1+\mathfrak{a}(\lambda)\big)\,, \tag{A.8}$$

and similarly $|\{\mu\}\rangle$ is the dominant right eigenvector of the α-twisted transfer matrix $t(\zeta,\kappa+\alpha)$ with eigenvalue

$$\Lambda(\zeta,\kappa+\alpha) = q^{\kappa+\alpha}a(\lambda)\left[\prod_{j=1}^{N/2}\frac{\mathrm{sh}(\lambda-\mu_j-\eta)}{\mathrm{sh}(\lambda-\mu_j)}\right]\big(1+\mathfrak{a}_\alpha(\lambda)\big) \tag{A.9}$$

Dividing (A.9) by (A.8) we obtain the identities

$$\rho(\zeta) = \frac{1+\mathfrak{a}_\alpha(\lambda)}{1+\mathfrak{a}(\lambda)}q^\alpha\phi(\lambda-\eta)\phi^{-1}(\lambda) = \frac{1+\overline{\mathfrak{a}}_\alpha(\lambda)}{1+\overline{\mathfrak{a}}(\lambda)}q^{-\alpha}\phi(\lambda+\eta)\phi^{-1}(\lambda) \tag{A.10}$$

which will be needed below. Here we have introduced the notation $\overline{\mathfrak{a}} = 1/\mathfrak{a}$ and $\overline{\mathfrak{a}}_\alpha = 1/\mathfrak{a}_\alpha$. In the derivation of the multiple integral formula below we shall use that ρ is analytic and non-zero inside the canonical contour $\mathcal{C}$ which follows from the Bethe equations and from the explicit form of the vacuum expectation values a and d.

The derivation of the density matrix for $\alpha = 0$ in [13] is divided into two steps. Step 1 is the derivation of the 'general left action' $\langle\{\lambda\}|T^{\alpha_1}_{\beta_1}(\xi_1,\kappa)\dots T^{\alpha_m}_{\beta_m}(\xi_m,\kappa)$ of a string of monodromy matrix elements on the left dominant eigenvector. This step remains the same as before. The general left action is given by Lemma 1 of [13]. In a second step one must calculate ratios of scalar products of the form

$$\chi = \frac{\langle\{\nu^+\}\cup\{\lambda^-\}|\{\mu\}\rangle}{\langle\{\lambda\}|\{\mu\}\rangle\prod_{j=1}^m \Lambda(\xi_j,\kappa)} \tag{A.11}$$

which are generated in step 1. A useful expression for these ratios in the untwisted case $\alpha = 0$ is provided by lemma 2 of [13]. This needs to be modified here.

The notation in (A.11) is meant as follows. We divide the sets $\{\lambda\}$ and $\{\nu\} = \{\nu_j\}_{j=1}^m = \{\ln\xi_j\}_{j=1}^m$ into disjoint subsets $\{\lambda^+\}$, $\{\lambda^-\}$ and $\{\nu^+\}$, $\{\nu^-\}$, such that their unions are $\{\lambda^+\}\cup\{\lambda^-\} = \{\lambda\}$ and $\{\nu^+\}\cup\{\nu^-\} = \{\nu\}$. The number of elements in a set $\{x\}$ will be denoted $|x|$. We shall assume that $|\lambda^+| = |\nu^+| = n$. For a given partition of $\{\lambda\}$ into $\{\lambda^+\}$, $\{\lambda^-\}$ we order the λs such that

$$(\lambda_1,\dots,\lambda_{N/2}) = (\lambda_1^+,\dots,\lambda_n^+,\lambda_1^-,\dots,\lambda_{N/2-n}^-) \tag{A.12}$$

and we define

$$(\widetilde{\lambda}_1,\dots,\widetilde{\lambda}_{N/2}) = (\nu_1^+,\dots,\nu_n^+,\lambda_1^-,\dots,\lambda_{N/2-n}^-)\,. \tag{A.13}$$

Then using lemma 2 of [14] (with the roles of λ and μ interchanged) we arrive after some trivial cancellations at

$$\begin{aligned}\chi = &\left[\prod_{j=1}^{|\nu^-|}\frac{\prod_{k=1}^{N/2} b(\lambda_k-\nu_j^-)}{a(\nu_j^-)(1+\mathfrak{a}(\nu_j^-))}\right]\left[\prod_{j=1}^{|\lambda^+|}\frac{\prod_{k=1,\lambda_k\neq\lambda_j^+}^{N/2} b(\lambda_k-\lambda_j^+)}{a(\lambda_j^+)(1+\mathfrak{a}(\nu_j^+))}\right]\det{}^{-1}_{|\lambda^+|}\left[\frac{c(\lambda_j^+-\nu_k^+)}{b(\lambda_j^+-\nu_k^+)}\right]\\ &\cdot\underbrace{\frac{\det_{N/2}\widehat{N}(\mu_j,\widetilde{\lambda}_k)}{\det_{N/2}\widehat{N}(\mu_j,\lambda_k)}\left[\prod_{j=1}^{|\lambda^+|}\phi(\nu_j^+-\eta)\phi^{-1}(\lambda_j^+-\eta)\right]}_{=\Xi},\end{aligned} \tag{A.14}$$

where

$$\widehat{N}(\mu_j,\lambda_k) = \mathrm{e}(\mu_j-\lambda_k) - \mathrm{e}(\lambda_k-\mu_j)\mathfrak{a}_\alpha(\lambda_k)\,. \tag{A.15}$$

In the following we concentrate on the term Ξ in the second line of (A.14). We want to transform it into a form that allows us to perform the Trotter limit $N\to\infty$. We define column vectors $\mathbf{u}_k$, $k = 1,\dots,|\nu^+| = n$, and $\mathbf{v}_k$, $k = 1,\dots,N/2$, by

$$\begin{aligned}(\mathbf{u}_k)^j &= \phi(\nu_k^+-\eta)\widehat{N}(\mu_j,\nu_k^+) = \phi(\nu_k^+-\eta)\big(\mathrm{e}(\mu_j-\nu_k^+) - \mathrm{e}(\nu_k^+-\mu_j)\mathfrak{a}_\alpha(\nu_k^+)\big)\,,\\ (\mathbf{v}_k)^j &= \phi(\lambda_k-\eta)\widehat{N}(\mu_j,\lambda_k) = \mathrm{e}(\mu_j-\lambda_k)\phi(\lambda_k-\eta) + q^{-2\alpha}\mathrm{e}(\lambda_k-\mu_j)\phi(\lambda_k+\eta)\,.\end{aligned} \tag{A.16}$$

In (A.16) we used the Bethe ansatz equations (A.3) to eliminate $q^{-2\kappa} d(\lambda_k)/a(\lambda_k)$. We have

$$\Xi = \frac{\det(\mathbf{u}_1, \dots, \mathbf{u}_n, \mathbf{v}_{n+1}, \dots, \mathbf{v}_{N/2})}{\det(\mathbf{v}_1, \dots, \mathbf{v}_{N/2})} \,. \tag{A.17}$$

Next we use a trick we learned from N. Kitanine [20] and which in a similar form originally appeared in [16]. Define a matrix X with matrix elements

$$X_l^j = q^\alpha \operatorname{cth}(\mu_l - \lambda_j) \operatorname{res}_{\lambda=\mu_l} \phi^{-1}(\lambda) \tag{A.18}$$

and column vectors $\mathbf{U}_k = \mathbf{U}(\nu_k^+) = X\mathbf{u}_k$, and $\mathbf{V}_k = X\mathbf{v}_k$. Then

$$\Xi = \frac{\det(\mathbf{U}_1, \dots, \mathbf{U}_n, \mathbf{V}_{n+1}, \dots, \mathbf{V}_{N/2})}{\det(\mathbf{V}_1, \dots, \mathbf{V}_{N/2})} \,. \tag{A.19}$$

The vectors $\mathbf{U}_k$ and $\mathbf{V}_k$ are easily calculated by means of the residue theorem. Choose two simple closed contours $\mathcal{C}_\lambda$ and $\mathcal{C}_\mu$ such that all Bethe roots λ_j are inside $\mathcal{C}_\lambda$ but outside $\mathcal{C}_\mu$ and all Bethe roots μ_j are inside $\mathcal{C}_\mu$ but outside $\mathcal{C}_\lambda$. Then

$$\begin{aligned}
&(\mathbf{V}_k)^j = \\
&\sum_{l=1}^{N/2} q^\alpha \operatorname{cth}(\mu_l - \lambda_j) \operatorname{res}_{\lambda=\mu_l} \phi^{-1}(\lambda) \big[\mathrm{e}(\mu_l - \lambda_k)\phi(\lambda_k - \eta) + q^{-2\alpha}\mathrm{e}(\lambda_k - \mu_l)\phi(\lambda_k + \eta)\big] \\
&\quad = \int_{\mathcal{C}_\mu} \frac{\mathrm{d}\mu}{2\pi\mathrm{i}} \underbrace{\operatorname{cth}(\mu - \lambda_j)\phi^{-1}(\mu)\big[q^\alpha \mathrm{e}(\mu - \lambda_k)\phi(\lambda_k - \eta) + q^{-\alpha}\mathrm{e}(\lambda_k - \mu)\phi(\lambda_k + \eta)\big]}_{= f(\mu)} \,.
\end{aligned} \tag{A.20}$$

The function f is periodic with period $\mathrm{i}\pi$, and $\lim_{\operatorname{Re}\mu\to\pm\infty} f(\mu) = 0$. Moreover, $\phi^{-1}(\mu)$ is analytic inside $\mathcal{C}_\lambda$. Hence, for $j \neq k$,

$$\begin{aligned}
(\mathbf{V}_k)^j &= -\int_{\mathcal{C}_\lambda} \frac{\mathrm{d}\mu}{2\pi\mathrm{i}} f(\mu) = -(\operatorname{res}_{\mu=\lambda_j} + \operatorname{res}_{\mu=\lambda_k} + \operatorname{res}_{\mu=\lambda_k+\eta} + \operatorname{res}_{\mu=\lambda_k-\eta}) f(\mu) \\
&= q^{-\alpha} \operatorname{cth}(\lambda_j - \lambda_k - \eta) - q^\alpha \operatorname{cth}(\lambda_j - \lambda_k + \eta) = K_\alpha(\lambda_j - \lambda_k) \,.
\end{aligned} \tag{A.21}$$

For $j = k$ we have a non-trivial residue from the second order pole at λ_j, and

$$(\mathbf{V}_j)^j = (q^{-\alpha}\phi(\lambda_j + \eta) - q^\alpha \phi(\lambda_j - \eta))\partial_\mu \phi^{-1}(\mu)\big|_{\mu=\lambda_j} + K_\alpha(0) \,. \tag{A.22}$$

Similarly, we obtain

$$\begin{aligned}
(\mathbf{U}_k)^j = q^\alpha \operatorname{cth}(\lambda_j - \nu_k^+)\phi^{-1}(\nu_k^+)\phi(\nu_k^+ - \eta)\big[1 + \mathfrak{a}_\alpha(\nu_k^+)\big] - q^\alpha \operatorname{cth}(\lambda_j - \nu_k^+ + \eta) \\
- q^\alpha \operatorname{cth}(\lambda_j - \nu_k^+ - \eta)\phi^{-1}(\nu_k^+ + \eta)\phi(\nu_k^+ - \eta)\mathfrak{a}_\alpha(\nu_k^+) \,.
\end{aligned} \tag{A.23}$$

Following once more [20] we eliminate the function ϕ from (A.22) and (A.23). This can be done by means of the identities (A.10). For the first term on the right hand

side of (A.22) we obtain

$$\big(q^{-\alpha}\phi(\lambda_j+\eta)-q^{\alpha}\phi(\lambda_j-\eta)\big)\partial_\mu\phi^{-1}(\mu)\big|_{\mu=\lambda_j}= \\ \lim_{\lambda\to\lambda_j}\big(q^{-\alpha}\phi(\lambda+\eta)-q^{\alpha}\phi(\lambda-\eta)\big)\frac{\mathfrak{a}'(\lambda)\phi^{-1}(\lambda)}{1+\mathfrak{a}(\lambda)}= \\ \lim_{\lambda\to\lambda_j}\mathfrak{a}'(\lambda)\rho(\zeta)\left[\frac{\overline{\mathfrak{a}}(\lambda)}{1+\overline{\mathfrak{a}}_\alpha(\lambda)}-\frac{1}{1+\mathfrak{a}_\alpha(\lambda)}\right]=-\mathfrak{a}'(\lambda_j)\rho(\zeta_j)\,, \quad \text{(A.24)}$$

where we used (A.10) in the second equation and the Bethe ansatz equation $\overline{\mathfrak{a}}(\lambda_j)=-1$ in the third equation. It follows that

$$(\mathbf{V}_k)^j=-\delta^j_k\mathfrak{a}'(\lambda_j)\rho(\zeta_j)+K_\alpha(\lambda_j-\lambda_k)\,. \quad \text{(A.25)}$$

Eliminating ϕ from (A.23) by means of (A.10) we end up with

$$(\mathbf{U}_k)^j=\operatorname{cth}(\lambda_j-\nu_k^+)(1+\mathfrak{a}(\nu_k^+))\rho(\xi_k^+) \\ -q^{\alpha}\operatorname{cth}(\lambda_j-\nu_k^++\eta)-q^{-\alpha}\operatorname{cth}(\lambda_j-\nu_k^+-\eta)\mathfrak{a}(\nu_k^+)\,. \quad \text{(A.26)}$$

From here on we can proceed as in [14]. Define a matrix $V=(\mathbf{V}_1,\dots,\mathbf{V}_{N/2})$ and a vector $\mathbf{W}(\nu)=V^{-1}\mathbf{U}(\nu)$. Then

$$\Xi=\det_{N/2}\big(V^{-1}\mathbf{U}_1,\dots,V^{-1}\mathbf{U}_n,\mathbf{e}_{n+1},\dots,\mathbf{e}_{N/2}\big)= \\ \det_n\big(\langle\mathbf{e}_j,V^{-1}\mathbf{U}_k\rangle\big)=\det_n\big(\mathbf{W}(\nu_k^+)^j\big)\,. \quad \text{(A.27)}$$

$\mathbf{W}(\nu_k^+)$ is the solution of the linear equation $V\mathbf{W}(\nu_k^+)=\mathbf{U}(\nu_k^+)$, or, explicitly,

$$\operatorname{cth}(\lambda_j-\nu_k^+)(1+\mathfrak{a}(\nu_k^+))\rho(\xi_k^+)-q^{\alpha}\operatorname{cth}(\lambda_j-\nu_k^++\eta)-q^{-\alpha}\operatorname{cth}(\lambda_j-\nu_k^+-\eta)\mathfrak{a}(\nu_k^+) \\ =-\mathbf{W}(\nu_k^+)^j\mathfrak{a}'(\lambda_j)\rho(\zeta_j)+\sum_{l=1}^{N/2}K_\alpha(\lambda_j-\lambda_l)\mathbf{W}(\nu_k^+)^l\,. \quad \text{(A.28)}$$

This can be transformed into a linear integral equation. For this purpose define

$$G(\lambda,\nu)=\frac{q^{\alpha}\operatorname{cth}(\lambda-\nu+\eta)}{1+\mathfrak{a}(\nu)}+\frac{q^{-\alpha}\operatorname{cth}(\lambda-\nu-\eta)}{1+\overline{\mathfrak{a}}(\nu)} \\ -\operatorname{cth}(\lambda-\nu)\rho(\xi)+\sum_{l=1}^{N/2}\frac{K_\alpha(\lambda-\lambda_l)\mathbf{W}(\nu)^l}{1+\mathfrak{a}(\nu)}\,. \quad \text{(A.29)}$$

This function is defined such that

$$G(\lambda_j,\nu_k^+)=\frac{\rho(\zeta_j)\mathfrak{a}'(\lambda_j)\mathbf{W}(\nu_k^+)^j}{1+\mathfrak{a}(\nu_k^+)}\,. \quad \text{(A.30)}$$

We shall assume that ν is located inside the canonical contour $\mathcal{C}$ shown in figure 1. By construction $G(\lambda,\nu)$ is then meromorphic inside $\mathcal{C}$ and has a single simple pole with

residue $-\rho(\xi)$ at $\lambda=\nu$. Using (A.30) it follows that

$$G(\lambda,\nu_k^+) = q^{-\alpha}\operatorname{cth}(\lambda-\nu_k^+-\eta) - \operatorname{cth}(\lambda-\nu_k^+)\rho(\xi_k^+) \\ + \int_{\mathcal{C}} \frac{\mathrm{d}\mu}{2\pi\mathrm{i}} \frac{G(\mu,\nu_k^+)K_\alpha(\lambda-\mu)}{\rho(\mathrm{e}^\mu)(1+\mathfrak{a}(\mu))} \tag{A.31}$$

which is a linear integral equation for G.

Combining (A.27) and (A.30) we infer that

$$\Xi = \left[\prod_{j=1}^{|\lambda^+|} \frac{1+\mathfrak{a}(\nu_j^+)}{\mathfrak{a}'(\lambda_j^+)\rho(\zeta_j^+)}\right] \det_{|\lambda^+|}\big(G(\lambda_j^+,\nu_k^+)\big)\,. \tag{A.32}$$

Inserting this into (A.14) we arrive at

$$\chi = \left[\prod_{j=1}^{|\nu^-|} \frac{\prod_{k=1}^{N/2} b(\lambda_k-\nu_j^-)}{a(\nu_j^-)(1+\mathfrak{a}(\nu_j^-))}\right] \left[\prod_{j=1}^{|\lambda^+|} \frac{\prod_{k=1,\lambda_k\neq\lambda_j^+}^{N/2} b(\lambda_k-\lambda_j^+)}{a(\lambda_j^+)\mathfrak{a}'(\lambda_j^+)\rho(\zeta_j^+)}\right] \frac{\det_{|\lambda^+|}\big(G(\lambda_j^+,\nu_k^+)\big)}{\det_{|\lambda^+|}\left[\frac{c(\lambda_j^+-\nu_k^+)}{b(\lambda_j^+-\nu_k^+)}\right]}\,. \tag{A.33}$$

This replaces the expression in lemma 2 of [13]. Comparing the two expressions we see only one explicit difference which is the appearance of the additional factor $\rho(\zeta_j^+)$ in the denominator. It always comes with a factor $\mathfrak{a}'(\lambda_j^+)$. Therefore it is easy to trace the modification required in the derivation of the multiple integral formula in [13]. There is, however, also an implicit change in the formula. The residue of $G(\lambda,\nu)$ at $\lambda=\nu$ is $-\rho(\xi)$ instead of -1. This causes another tiny modification in the derivation of the multiple integral formula. In the first equation (65) of [13] additional $m-|\lambda^+|$ factors of ρ^{-1} appear which together with the $|\lambda^+|$ explicit factors gives exactly one factor per integral. The final result for the density matrix matrix is

$$\frac{\langle\kappa|T_{\beta_1}^{\alpha_1}(\xi_1,\kappa)\dots T_{\beta_m}^{\alpha_m}(\xi_m,\kappa)|\kappa+\alpha\rangle}{\langle\kappa|\prod_{j=1}^m t(\xi_j,\kappa)|\kappa+\alpha\rangle} \\ = \left[\prod_{j=1}^{|\alpha^+|}\int_{\mathcal{C}}\frac{\mathrm{d}\mu_j}{2\pi\mathrm{i}}\frac{F_j(\mu_j)}{\rho(\mathrm{e}^{\mu_j})(1+\mathfrak{a}(\mu_j))}\right]\left[\prod_{j=|\alpha^+|+1}^{m}\int_{\mathcal{C}}\frac{\mathrm{d}\mu_j}{2\pi\mathrm{i}}\frac{\overline{F}_j(\mu_j)}{\rho(\mathrm{e}^{\mu_j})(1+\overline{\mathfrak{a}}(\mu_j))}\right] \\ \frac{\det[-G(\mu_j,\nu_k)]}{\prod_{1\le j<k\le m}\operatorname{sh}(\mu_j-\mu_k-\eta)\operatorname{sh}(\nu_k-\nu_j)}\,, \tag{A.34}$$

where we have used the notation of [13], i.e.

$$F_j(\lambda) = \prod_{k=1}^{x_j-1}\operatorname{sh}(\lambda-\nu_k-\eta)\prod_{k=x_j+1}^{m}\operatorname{sh}(\lambda-\nu_k)\,, \quad j=1,\dots,|\alpha^+|\,, \tag{A.35a}$$

$$\overline{F}_j(\lambda) = \prod_{k=1}^{x_j-1}\operatorname{sh}(\lambda-\nu_k+\eta)\prod_{k=x_j+1}^{m}\operatorname{sh}(\lambda-\nu_k)\,, \quad j=|\alpha^+|+1,\dots,m\,, \tag{A.35b}$$

and for $j = 1,\dots,|\alpha^+|$ we define x_j to be the position of the $(|\alpha^+| - j + 1)$th '+' in the sequence of upper indices $(\alpha_j)_{j=1}^m$ while for $j = |\alpha^+| + 1,\dots,m$ it means the position of the $(j - |\alpha^+|)$th '−' in the sequence of lower indices $(\beta_j)_{j=1}^m$.

Finally we replace ξ_k by ξ_{m-k+1} and define $\varepsilon_k = \alpha_{m-k+1}$, $\varepsilon'_k = \beta_{m-k+1}$ for $k = 1,\dots,m$. We denote the position of the jth '+' in $(\varepsilon_j)_{j=1}^m$ by ε_j^+, the position of the jth '−' in $(\varepsilon'_j)_{j=1}^m$ by ε_j^-. Then

$$x_j = \begin{cases} m - \varepsilon_j^+ + 1 & j = 1,\dots,p \\ m - \varepsilon_{m-j+1}^- + 1 & j = p+1,\dots,m \end{cases}, \tag{A.36}$$

where $p = |\alpha^+|$. Defining

$$\ell_j = \begin{cases} \varepsilon_j^+ & j = 1,\dots,p \\ \varepsilon_{m-j+1}^- & j = p+1,\dots,m \end{cases}, \tag{A.37}$$

we obtain $x_j = m - \ell_j + 1$, $j = 1,\dots,m$. Finally, setting $F_{\ell_j}^+(\mu) = F_j(\mu)$ and $F_{\ell_j}^-(\mu) = \overline{F}_j(\mu)$ and using (A.1), we arrive at (29).

Appendix B: Relation with previous results

In our previous work [2,4], before we knew the multiple integral representation for finite α, we conjectured formulae which we claimed to hold in the limit $\alpha \to 0$, relevant for the physical correlation functions of the XXZ chain. We introduced a function, say, $\omega_{\mathrm{old}}(\mu_1,\mu_2;\alpha)$ defined by an integral formula involving, among other functions, a function G_{old} which is different from G defined in (31). Here we explain why our previous results remain unaltered in the limit $\alpha \to 0$ if we replace $\omega_{\mathrm{old}}(\mu_1,\mu_2;\alpha)$ with $-\omega(\xi_1,\xi_2|\kappa,\alpha) + \omega_0(\xi|\alpha)$ (the minus sign is due to a change of conventions in which we followed [9,19]).

Our previous ad hoc definitions were

$$\omega_{\mathrm{old}}(\nu_1,\nu_2;\alpha) - \omega_0(\xi|\alpha) = -\xi^\alpha \Psi_{\mathrm{old}}(\nu_2,\nu_1;-\alpha) + \Delta\psi(\xi)\,, \tag{B.1}$$

$$\Psi_{\mathrm{old}}(\nu_2,\nu_1;-\alpha) = 2\int_{\mathcal{C}} \mathrm{d}m_0(\mu) G_{\mathrm{old}}(\mu,\nu_2;-\alpha)\big(q^\alpha \operatorname{cth}(\mu - \nu_1 - \eta) - \operatorname{cth}(\mu - \nu_1)\big)\,,$$

where $\mathrm{d}m_0(\mu) = \mathrm{d}m(\mu)|_{\alpha=0}$ and where G_{old} was the solution of the linear integral equation

$$G_{\mathrm{old}}(\lambda,\nu;-\alpha) = q^{-\alpha} \operatorname{cth}(\lambda - \nu - \eta) - \operatorname{cth}(\lambda - \nu) + \int_{\mathcal{C}} \mathrm{d}m_0(\mu) K_\alpha(\lambda - \mu) G(\mu,\nu;-\alpha)\,. \tag{B.2}$$

Comparing with (52), (50) and (31) we see that apart from some conventional sign changes the only difference is that the function ρ is replaced by unity in the old definitions. Using that $\omega_0(\xi|0) = 0$ we conclude in particular that

$$\omega(\xi_1,\xi_2|\kappa,0) = -\omega_{\mathrm{old}}(\nu_1,\nu_2;0) \tag{B.3}$$

and that $G(\lambda,\nu)|_{\alpha=0} = G_{\mathrm{old}}(\lambda,\nu;0) = G_0(\lambda,\nu)$ which satisfies the integral equation

$$G_0(\lambda,\nu) = \mathrm{e}(\nu-\lambda) + \int_{\mathcal{C}} \mathrm{d}m_0(\mu) K(\lambda-\mu) G_0(\mu,\nu)\,. \tag{B.4}$$

This integral equation implies the symmetry

$$\omega(\xi_1,\xi_2|\kappa,0) = \omega(\xi_2,\xi_1|\kappa,0)\,. \tag{B.5}$$

Let us define

$$\omega'(\xi_1,\xi_2) = \partial_\alpha\big(\xi^{-\alpha}\omega(\xi_1,\xi_2|\kappa,\alpha)\big)\big|_{\alpha=0}\,, \tag{B.6a}$$

$$\omega'_{\mathrm{old}}(\nu_1,\nu_2) = \partial_\alpha\big(\xi^{-\alpha}\omega_{\mathrm{old}}(\nu_1,\nu_2;\alpha)\big)\big|_{\alpha=0}\,. \tag{B.6b}$$

We shall show below that

$$\omega'_{\mathrm{old}}(\nu_1,\nu_2) = \tfrac{1}{2}\big(\omega'(\xi_2,\xi_1) - \omega'(\xi_1,\xi_2)\big)\,. \tag{B.7}$$

Accepting this for a moment let us insert $-\omega+\omega_0$ instead of ω_{old} into our previous formula for the exponential form, e.g. into equation (35) of [2], which actually means to use (80) for the **t** independent part of the exponential form. Then using (B.3), (B.5) and (B.7) and the fact that $\xi^{-\alpha}\omega_0(\xi|\alpha) = \mathcal{O}(\alpha^2)$ we recover our previous result, namely equation (37) of [2], in the limit $\alpha \to 0$.

It remains to prove (B.7). For this purpose consider

$$\begin{aligned}
\tfrac{1}{2}\big(\omega'_{\mathrm{old}}(\nu_1,\nu_2) + \omega'(\xi_1,\xi_2)\big) &= \big(\rho'(\xi_1) - \rho'(\xi_2)\big)\psi(\xi) \\
&- \rho'(\xi_1)\int_{\mathcal{C}} \mathrm{d}m_0(\mu) G_0(\mu,\nu_2)\,\mathrm{cth}(\mu-\nu_1) - \int_{\mathcal{C}} \mathrm{d}m_0(\mu)\rho'(\mathrm{e}^{\mu}) G_0(\mu,\nu_2)\mathrm{e}(\nu_1-\mu) \\
&+ \int_{\mathcal{C}} \mathrm{d}m_0(\mu) G'(\mu,\nu_2)\mathrm{e}(\nu_1-\mu)\,,
\end{aligned} \tag{B.8}$$

where $\rho'(\xi) = \partial_\alpha\rho(\xi)|_{\alpha=0}$, and $G'(\mu,\nu_2) = \partial_\alpha(G(\mu,\nu_2) + G_{\mathrm{old}}(\lambda,\nu;\alpha))|_{\alpha=0}$. Taking the α-derivative of (31) and (B.2) we find

$$\begin{aligned}
G'(\lambda,\nu_2) = -\rho'(\xi_2)\,\mathrm{cth}(\lambda-\nu_2) &- \int_{\mathcal{C}} \mathrm{d}m_0(\mu)\rho'(\mathrm{e}^{\mu}) G_0(\mu,\nu_2) K(\lambda-\mu) \\
&- \int_{\mathcal{C}} \mathrm{d}m_0(\mu) K(\lambda-\mu) G'(\mu,\nu_2)\,.
\end{aligned} \tag{B.9}$$

Using (B.4) and (B.9) we can eliminate G' from (B.8) by means of the 'dressed function trick'. We arrive at

$$\begin{aligned}
\tfrac{1}{2}\big(\omega'_{\mathrm{old}}(\nu_1,\nu_2) + \omega'(\xi_1,\xi_2)\big) &= \big(\rho'(\xi_1) - \rho'(\xi_2)\big)\psi(\xi) \\
&- \rho'(\xi_1)\int_{\mathcal{C}} \mathrm{d}m_0(\mu) G_0(\mu,\nu_2)\,\mathrm{cth}(\mu-\nu_1) - \rho'(\xi_2)\int_{\mathcal{C}} \mathrm{d}m_0(\mu) G_0(\mu,\nu_1)\,\mathrm{cth}(\mu-\nu_2) \\
&- \int_{\mathcal{C}} \mathrm{d}m_0(\mu)\rho'(\mathrm{e}^{\mu}) G_0(\mu,\nu_1) G_0(\mu,\nu_2)
\end{aligned} \tag{B.10}$$

which is obviously symmetric. Then (B.7) follows if one takes into account that $\omega'_{\mathrm{old}}(\xi_1,\xi_2)$ is antisymmetric, which was shown in [4].

Now let us discuss how the operators $\mathbf{t}_j$ described in the section 7 are related to the operators $\mathbf{h}_j$ (see formulae (40)-(42) of [2]) in the limit $\alpha\to 0$. As we mentioned above the operators $\mathbf{t}_j$ have a pole of first order when $\alpha\to 0$. On the other hand, it follows from the formula (92) that the density matrix depends only on the combination $(\rho_j-1)\mathbf{t}_j$. Since $\lim_{\alpha\to 0}\rho_j=1$, $1-\rho_j=\mathcal{O}(\alpha)$, and one obtains for $(\rho_j-1)\mathbf{t}_j$ a finite result in the limit $\alpha\to 0$. So we actually need only the residues of $\mathbf{t}_j$. Let us define

$$\mathbf{t}_j^{(0)}=\lim_{\alpha\to 0}(1-q^{\alpha})\mathbf{t}_j\,. \tag{B.11}$$

Since for the moment we do not have an explicit formula for $\mathbf{t}_j$ in the general case, let us describe the relation with $\mathbf{h}_j$ again only for the cases $m=1,2$ where we know the explicit result (93) and (94), (95). It is enough to consider $j=1$.

For $m=1$

$$\mathbf{t}^{(0)}_{1[1,1]}=-\mathbf{h}_{1[1,1]}=-\frac{1}{2}\,I\otimes\sigma_1^z\,. \tag{B.12}$$

For $m=2$ we simply get from (94)

$$\mathbf{t}^{(0)}_{1[1,2]}=-\frac{1}{4}\,I\otimes\left[\sigma_1^z-\frac{q-q^{-1}}{\xi_1/\xi_2-\xi_2/\xi_1}\cdot(\sigma_1^+\sigma_2^--\sigma_1^-\sigma_2^+)\right] \tag{B.13}$$

and

$$\begin{aligned}&\mathbf{t}^{(0)}_{1[1,2]}+\mathbf{h}_{1[1,2]}\\&\quad=-\frac{1}{4}\,\frac{\xi_1/\xi_2+\xi_2/\xi_1}{\xi_1/\xi_2-\xi_2/\xi_1}\sigma_2^z\otimes\left[\sigma_1^z\sigma_2^z-\frac{q+q^{-1}}{\xi_1/\xi_2+\xi_2/\xi_1}\cdot(\sigma_1^+\sigma_2^-+\sigma_1^-\sigma_2^+)\right].\end{aligned} \tag{B.14}$$

It is interesting to note the following. In spite of the fact that the operators $\mathbf{h}_j$ are fermionic and the $\mathbf{t}_j$ are bosonic, the limit of the α-trace of the corresponding exponentials should coincide

$$\lim_{\alpha\to 0}\ \mathbf{tr}^{\alpha}\big\{\exp\big(\sum_j\log\rho_j\,\mathbf{t}_j\big)-\exp\big(-\sum_j\varphi_j\mathbf{h}_j\big)\big\}\big(q^{2\alpha S(0)}\mathcal{O}\big)=0 \tag{B.15}$$

where $\varphi_j=\varphi(\xi_j|\kappa,0)$. We do not have a complete understanding of this relation for the moment, but we can follow how it works for $m=1,2$. The case $m=1$ is trivial while the case $m=2$ is more interesting. For instance, one could expect that terms containing $\varphi_1\varphi_2$ appear, but they do not. For the fermionic formula this is a simple consequence of the anti-commutation relations of the operators $\mathbf{h}_j$. The reason why do they not appear for the bosonic formula is different, namely, because of the relation $\mathbf{t}_1^{(0)}\mathbf{t}_2^{(0)}=0$, which can be checked. We plan to study this point more carefully in the future.

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